Supporting Information

Mechanistic Investigation of the Pyrolysis of Brown Grease

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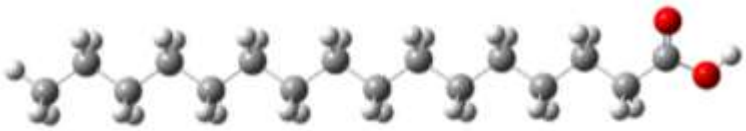
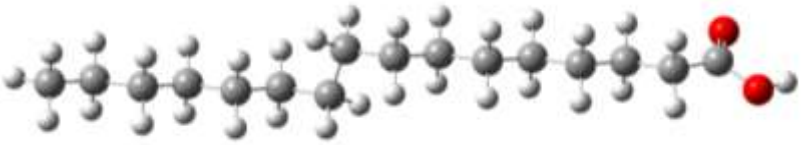
Contents:

Figure S1. Conformers for Palmitic Acid. The most stable conformer is R1.



R1



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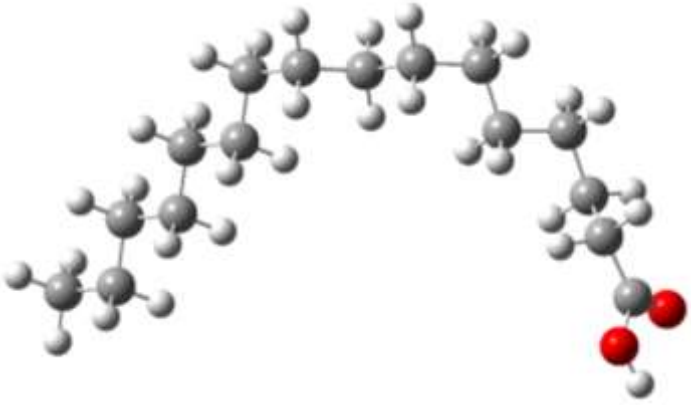

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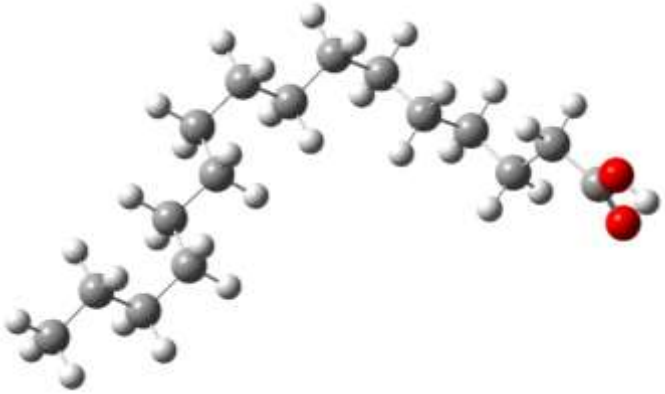

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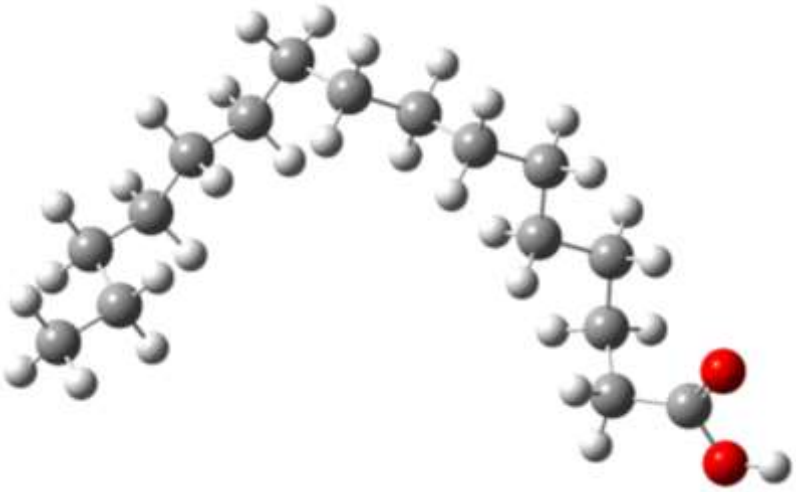

R5

Coordinates

The pyrolysis reaction: (Pathway A1) (Reactant RA1)

Basis set = 6-31G(d)
Nuclear repulsion energy= 1185.396506 Hartrees
E(RB3LYP) = -779.448022 Hartrees
Formula: C16H32O2
Cartesian:

C	-8.61542800	0.06157600	0.09378500
O	-9.40409200	-0.17841300	0.98096200
O	-8.79733100	1.09004100	-0.77796000
H	-9.63005000	1.52200700	-0.50961600
C	-7.33167000	-0.68631600	-0.18519700
H	-7.33429300	-1.00335400	-1.23575000
H	-7.33550400	-1.58126200	0.44310300
C	-6.07668500	0.16710500	0.08817300
H	-6.10892900	1.06467500	-0.54130800
H	-6.09712300	0.51315200	1.13060900
C	-4.77648600	-0.60425000	-0.16989100
H	-4.75812700	-1.50772900	0.45702600
H	-4.76401600	-0.95593300	-1.21216600
C	-3.51637500	0.22792900	0.10092800
H	-3.53713600	1.13197500	-0.52539600
H	-3.53132300	0.58006500	1.14293900
C	-2.21212600	-0.53791000	-0.15662900
H	-2.19813900	-0.89093700	-1.19853700
H	-2.19250200	-1.44204100	0.46986300
C	-0.95093100	0.29288800	0.11349800
H	-0.96575200	0.64671400	1.15513000
H	-0.97060500	1.19674800	-0.51347000
C	0.35377100	-0.47262500	-0.14254300
H	0.36822000	-0.82701800	-1.18404200
H	0.37328000	-1.37627500	0.48477200
C	1.61524600	0.35795700	0.12699600
H	1.60028100	0.71299600	1.16826400
H	1.59598900	1.26127500	-0.50083600
C	2.92005300	-0.40779700	-0.12782100
H	2.93487100	-0.76315200	-1.16900400
H	2.93921900	-1.31096800	0.50023200
C	4.18166800	0.42266100	0.14144600
H	4.16651400	0.77848600	1.18246000
H	4.16278900	1.32556600	-0.48701500
C	5.48643400	-0.34346000	-0.11245900
H	5.50155700	-0.69939100	-1.15344200
H	5.50519400	-1.24631400	0.51606600
C	6.74819100	0.48677500	0.15678900
H	6.73285300	0.84298100	1.19770700
H	6.72962300	1.38949300	-0.47200400
C	8.05294800	-0.27924400	-0.09642900

H	8.06946100	-0.63551400	-1.13742300
H	8.07254200	-1.18211500	0.53229600
C	9.31499500	0.55041800	0.17285000
H	9.29910500	0.90585800	1.21308500
H	9.29610000	1.45215800	-0.45579100
C	10.61311200	-0.22235300	-0.08243000
H	10.67464600	-0.56080100	-1.12418500
H	11.49484700	0.39686200	0.11883100
H	10.67749300	-1.11136000	0.55717600

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The pyrolysis reaction: (Pathway A1) (Transition state, TS Ketene, TSA1)

Basis set = 6-31G(d)

Nuclear repulsion energy= 1183.845617 Hartrees

E(RB3LYP) = -779.318052 Hartrees

Formula: C16H32O2

Cartesian:

C	-8.60993200	-0.09546600	0.05098400
O	-9.75996100	-0.28959600	0.17529500
O	-8.10589400	1.68996100	0.02298200
H	-8.83835900	2.12484900	-0.44982800
C	-7.35022500	-0.47571900	-0.45802600
H	-7.50693400	0.91749600	-0.77047100
H	-7.41354500	-1.41294900	-1.01709400
C	-6.09202500	-0.34923300	0.41519300
H	-6.15646200	0.55850800	1.02464900
H	-6.04110000	-1.19517000	1.11667600
C	-4.81159700	-0.31833800	-0.42947100
H	-4.78269100	-1.20377600	-1.08173200
H	-4.84398400	0.55259900	-1.09897500
C	-3.53481500	-0.27078700	0.41901400
H	-3.50912400	-1.14402300	1.08777300
H	-3.56734100	0.61224800	1.07423500
C	-2.24822600	-0.23506800	-0.41609600
H	-2.21697800	-1.11747300	-1.07253100
H	-2.27359600	0.63860800	-1.08413700
C	-0.96964500	-0.18820500	0.43052400
H	-0.94447500	-1.06204800	1.09857100
H	-1.00155600	0.69388400	1.08725100
C	0.31723300	-0.15174200	-0.40399300
H	0.34883300	-1.03370600	-1.06105200
H	0.29191600	0.72222000	-1.07187900
C	1.59609800	-0.10505700	0.44226200
H	1.62137500	-0.97905500	1.11013200
H	1.56435200	0.77681400	1.09938700
C	2.88306700	-0.06835900	-0.39211600
H	2.91468000	-0.95016800	-1.04938600
H	2.85777100	0.80571600	-1.05988800
C	4.16200300	-0.02183500	0.45404000
H	4.18727800	-0.89591700	1.12181200
H	4.13035200	0.85994800	1.11132000

C	5.44898100	0.01491500	-0.38031600
H	5.48057900	-0.86684200	-1.03764900
H	5.42370500	0.88902700	-1.04804200
C	6.72796300	0.06136500	0.46576100
H	6.75319200	-0.81275200	1.13353800
H	6.69635400	0.94316800	1.12307200
C	8.01501200	0.09806500	-0.36816500
H	8.04775200	-0.78373800	-1.02561300
H	7.99089700	0.97222800	-1.03610100
C	9.29420200	0.14455100	0.47748700
H	9.31888200	-0.72909000	1.14444400
H	9.26213400	1.02597100	1.13381000
C	10.57452100	0.18087100	-0.36328100
H	11.46908600	0.21369300	0.26923500
H	10.65270500	-0.70559500	-1.00488900
H	10.59545600	1.06265900	-1.01566600

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The pyrolysis reaction: (Pathway A1) (ketene product)

Basis set = 6-31G(d)
Nuclear repulsion energy= 1220.629988 Hartrees
E(RB3LYP) = -779.321731 Hartrees
Formula: C16H32O2
Cartesian:

C	7.85595000	0.40868900	0.45929500
O	7.99339800	1.52354800	0.82128800
O	5.95253500	2.82367100	-0.96581300
H	6.81080300	2.69569200	-0.52940900
C	7.69866600	-0.83010900	0.05587600
H	5.38540000	3.14894300	-0.25073300
H	8.61130700	-1.39448500	-0.11757300
C	6.34589100	-1.46778600	-0.21750100
H	6.28527100	-2.41351700	0.33954600
H	6.29645600	-1.73633800	-1.28266300
C	5.14664400	-0.57930100	0.13966400
H	5.17331600	-0.35751900	1.21685900
H	5.23631400	0.38342500	-0.38270500
C	3.80263300	-1.23007300	-0.21009500
H	3.77691700	-1.45133400	-1.28714100
H	3.71912900	-2.19966700	0.30343200
C	2.59454800	-0.35747400	0.15453800
H	2.68165200	0.61163600	-0.35813500
H	2.61883800	-0.13591000	1.23205700
C	1.24693500	-0.99939500	-0.19959500
H	1.22284800	-1.22061300	-1.27697100
H	1.16144800	-1.97022200	0.31111800
C	0.03842200	-0.12743700	0.16502200
H	0.12461200	0.84335300	-0.34540100
H	0.06235900	0.09384900	1.24258000
C	-1.30970500	-0.76791700	-0.19012400

H	-1.33357700	-0.98896500	-1.26763600
H	-1.39579900	-1.73904800	0.31988600
C	-2.51822200	0.10408400	0.17443700
H	-2.43178500	1.07524000	-0.33536400
H	-2.49444500	0.32503800	1.25204000
C	-3.86648200	-0.53583200	-0.18124900
H	-3.89019400	-0.75672300	-1.25883000
H	-3.95297700	-1.50707500	0.32847600
C	-5.07492300	0.33632500	0.18318000
H	-4.98822100	1.30758600	-0.32640300
H	-5.05130700	0.55712200	1.26080600
C	-6.42327000	-0.30320800	-0.17283900
H	-6.44679500	-0.52404800	-1.25047400
H	-6.51005500	-1.27449300	0.33680800
C	-7.63174300	0.56876100	0.19120400
H	-7.54595100	1.54029200	-0.31833300
H	-7.60938900	0.78979600	1.26894800
C	-8.98030000	-0.07018000	-0.16481300
H	-9.00316900	-0.29045800	-1.24167600
H	-9.06667600	-1.04049200	0.34483500
C	-10.18140700	0.80745500	0.20197400
H	-10.14179700	1.77170500	-0.31979000
H	-11.12813300	0.32362500	-0.06453300
H	-10.20569400	1.01624500	1.27873800

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The pyrolysis reaction: (Pathway A) (ketene + palmitic acid)

Basis set = 6-31G(d)
Nuclear repulsion energy= 3146.523687 Hartrees
E(RB3LYP) = -1482.477464 Hartrees
Formula: C32H62O3
Cartesian:

C	-0.42494400	7.36583600	-2.01118800
O	-0.74161100	8.35626900	-1.44945600
C	-0.07329900	6.27275000	-2.64310900
H	-0.02622300	6.33714400	-3.72748800
C	0.27775000	4.97391500	-1.93595200
H	0.00193100	5.05275700	-0.88000800
H	-0.34734900	4.17430800	-2.35786500
C	-2.65645700	6.84818600	1.01194600
O	-1.75846700	6.12314500	0.62615500
O	-2.90670500	8.05865300	0.47795600
H	-2.23568200	8.22274500	-0.22039200
C	-3.60451100	6.53447400	2.15341800
H	-4.61385600	6.84485000	1.85617400
H	-3.32366200	7.19914500	2.98248300
C	-3.57187300	5.06924400	2.59912000
H	-4.10471600	4.98596600	3.55576100
H	-2.53105200	4.78093800	2.78924900
C	1.76072800	4.59089400	-2.07628400

H	2.02744900	4.54271700	-3.14220300
H	2.37906300	5.38821700	-1.64214100
C	2.09179000	3.25209700	-1.40404500
H	1.46271700	2.46105300	-1.83894900
H	1.82001100	3.30459100	-0.33955600
C	3.56776500	2.85319500	-1.53233600
H	3.83847500	2.79939100	-2.59738600
H	4.19647800	3.64536500	-1.09954400
C	3.90057600	1.51656400	-0.85666200
H	3.62972500	1.57149400	0.20821400
H	3.27059100	0.72467100	-1.28860700
C	5.37592800	1.11524400	-0.98364500
H	5.64642700	1.05823200	-2.04862200
H	6.00595800	1.90805400	-0.55353000
C	5.70840900	-0.21970100	-0.30454700
H	5.07761900	-1.01234900	-0.73396700
H	5.43814100	-0.16193600	0.76041200
C	7.18334600	-0.62269500	-0.43102500
H	7.45339400	-0.68224300	-1.49597600
H	7.81425800	0.17056800	-0.00297300
C	7.51523400	-1.95640800	0.25077400
H	6.88387200	-2.74957400	-0.17685100
H	7.24529400	-1.89636100	1.31571200
C	8.98990000	-2.36049800	0.12470500
H	9.25971400	-2.42178000	-0.94020200
H	9.62135400	-1.56694300	0.55142300
C	9.32135400	-3.69337900	0.80832700
H	8.68966500	-4.48690100	0.38177900
H	9.05150800	-3.63180700	1.87323600
C	10.79564300	-4.09835800	0.68284200
H	11.06633200	-4.16119900	-0.38189700
H	11.42827600	-3.30533100	1.10916700
C	11.12725600	-5.43076400	1.36719000
H	10.49584600	-6.22340000	0.94087300
H	10.85753400	-5.36791600	2.43114100
C	12.60139000	-5.82755800	1.23717000
H	12.80544300	-6.78211200	1.73576200
H	12.89220500	-5.93283100	0.18458200
H	13.25668200	-5.07072000	1.68592100
C	-4.19333400	4.10016000	1.58451700
H	-5.23448700	4.39830400	1.38814800
H	-3.65759300	4.18728500	0.63065000
C	-4.16458100	2.63934300	2.05135500
H	-4.69166600	2.55275600	3.01352300
H	-3.12349300	2.34351900	2.24775400
C	-4.78652500	1.66358100	1.04402100
H	-5.82802900	1.95908700	0.84751600
H	-4.26015800	1.75221800	0.08208800
C	-4.75420600	0.20105900	1.50631300
H	-3.71275300	-0.09421000	1.70300600

H	-5.28046800	0.11263700	2.46853500
C	-5.37514400	-0.77490200	0.49846100
H	-6.41668500	-0.47973400	0.30181100
H	-4.84900900	-0.68611900	-0.46376700
C	-5.34232700	-2.23770800	0.95993600
H	-4.30083300	-2.53273300	1.15696900
H	-5.86885600	-2.32669500	1.92193300
C	-5.96251100	-3.21354000	-0.04851500
H	-7.00403800	-2.91857200	-0.24549600
H	-5.43602000	-3.12435900	-1.01052500
C	-5.92953200	-4.67647100	0.41254200
H	-4.88803500	-4.97138400	0.60976000
H	-6.45629000	-4.76580000	1.37437800
C	-6.54930700	-5.65213400	-0.59631500
H	-7.59079700	-5.35721900	-0.79353300
H	-6.02253700	-5.56274100	-1.55814400
C	-6.51636700	-7.11513400	-0.13550400
H	-5.47486100	-7.41003300	0.06183600
H	-7.04329100	-7.20457800	0.82626100
C	-7.13582300	-8.09088100	-1.14420600
H	-8.17763700	-7.79695900	-1.34196800
H	-6.60914300	-8.00251800	-2.10633600
C	-7.10322600	-9.55395700	-0.68382800
H	-6.06237800	-9.84812900	-0.48687700
H	-7.63011600	-9.64268500	0.27700700
C	-7.72372600	-10.52125600	-1.69711800
H	-7.68505600	-11.55654300	-1.33920600
H	-8.77535900	-10.27413300	-1.88841900
H	-7.19582200	-10.48119300	-2.65801200

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The pyrolysis reaction: (Pathway A1) (the reactant, RA1)

Basis set = 6-31G(d)
Nuclear repulsion energy= 1177.4703663Hartrees
E(RM062X) = -779.080448 Hartrees
Formula: C16H32O2
Cartesian:

C	8.56451600	-0.05850500	0.08135600
O	9.44288900	0.28600700	0.83043700
O	8.63657700	-1.20301500	-0.63357300
H	9.48627500	-1.61599400	-0.40068500
C	7.27980800	0.68419400	-0.18388400
H	7.28488500	1.00303500	-1.23348400
H	7.28828200	1.57838200	0.44368400
C	6.03558600	-0.17069300	0.08171600
H	6.06502300	-1.05803400	-0.56017700
H	6.05549900	-0.53016000	1.11849900
C	4.74444400	0.60662100	-0.16310400
H	4.72686300	1.49861200	0.47810700
H	4.73100300	0.97200100	-1.19948600

C	3.49240100	-0.22854200	0.09583800
H	3.51230200	-1.12120600	-0.54457000
H	3.50723900	-0.59385000	1.13206500
C	2.19709100	0.54218600	-0.15016300
H	2.18287800	0.90830800	-1.18625900
H	2.17789900	1.43485600	0.49051700
C	0.94450000	-0.29246200	0.10808800
H	0.95924900	-0.65904600	1.14402000
H	0.96398300	-1.18506900	-0.53273300
C	-0.35159800	0.47720300	-0.13704400
H	-0.36622600	0.84415700	-1.17288700
H	-0.37112200	1.36965400	0.50402400
C	-1.60408300	-0.35770500	0.12092000
H	-1.58902900	-0.72502200	1.15662900
H	-1.58461300	-1.25001500	-0.52037400
C	-2.90056600	0.41160100	-0.12332700
H	-2.91584000	0.77877900	-1.15909400
H	-2.91986900	1.30400500	0.51784500
C	-4.15291300	-0.42333200	0.13522500
H	-4.13729800	-0.79071700	1.17091800
H	-4.13377200	-1.31564700	-0.50609200
C	-5.44957400	0.34591300	-0.10826600
H	-5.46563900	0.71272000	-1.14415300
H	-5.46828300	1.23858200	0.53255900
C	-6.70189700	-0.48866300	0.15160300
H	-6.68554400	-0.85546600	1.18752300
H	-6.68325000	-1.38138800	-0.48920700
C	-7.99867200	0.28026300	-0.09134400
H	-8.01640900	0.64636800	-1.12761000
H	-8.01750100	1.17376800	0.54856900
C	-9.25150900	-0.55344700	0.17026400
H	-9.23214600	-0.91766800	1.20554500
H	-9.23100400	-1.44528000	-0.46932200
C	-10.53945400	0.22790000	-0.07678200
H	-10.59119300	0.57652700	-1.11371100
H	-11.42566100	-0.38339200	0.11636100
H	-10.59117400	1.10909100	0.57149400

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The pyrolysis reaction: (Pathway A1) (Ketene Transition State, TSA1)

Basis set = 6-31G(d)

Nuclear repulsion energy= 1176.731970 Hartrees

E(RM062X) = -778.944691 Hartrees

Formula: C16H32O2

Cartesian:

C	-8.54831800	-0.04509400	0.03038400
O	-9.70400700	-0.20719200	0.12706700
O	-8.03808200	1.63533300	-0.03861600
H	-8.76029800	2.10007100	-0.49415200
C	-7.30074400	-0.52459500	-0.41994100

H	-7.44032300	0.89182300	-0.80089600
H	-7.38936000	-1.49891400	-0.89937200
C	-6.05247900	-0.34062800	0.44212900
H	-6.11821700	0.60035800	0.99909400
H	-5.99171100	-1.14317700	1.19008300
C	-4.77942400	-0.34852700	-0.40262600
H	-4.75131000	-1.26210700	-1.01268700
H	-4.81245000	0.49160000	-1.10924900
C	-3.51031800	-0.26282400	0.44160800
H	-3.48182000	-1.10761600	1.14393100
H	-3.54393100	0.64676200	1.05749600
C	-2.23327800	-0.25963200	-0.39602400
H	-2.20114200	-1.16845900	-1.01314400
H	-2.26067500	0.58590500	-1.09742600
C	-0.96239900	-0.17595300	0.44667400
H	-0.93537700	-1.02124200	1.14852300
H	-0.99459300	0.73302200	1.06351900
C	0.31473300	-0.17351400	-0.39073100
H	0.34688000	-1.08270400	-1.00735400
H	0.28742500	0.67151000	-1.09291200
C	1.58590800	-0.08931300	0.45150100
H	1.61289700	-0.93393800	1.15417400
H	1.55404100	0.82020900	1.06761900
C	2.86306800	-0.08782400	-0.38587600
H	2.89519000	-0.99769700	-1.00149700
H	2.83574200	0.75638900	-1.08904800
C	4.13430300	-0.00263600	0.45616500
H	4.16142800	-0.84653900	1.15971100
H	4.10233900	0.90750400	1.07138800
C	5.41148500	-0.00178200	-0.38117400
H	5.44392100	-0.91239000	-0.99568200
H	5.38390100	0.84155000	-1.08538900
C	6.68271300	0.08489800	0.46074600
H	6.71008100	-0.75816100	1.16533600
H	6.65027700	0.99578200	1.07489800
C	7.96000000	0.08531200	-0.37614800
H	7.99387200	-0.82612000	-0.98961900
H	7.93281000	0.92760500	-1.08185100
C	9.23166400	0.17398900	0.46536200
H	9.25707300	-0.66756400	1.16962900
H	9.19619300	1.08494400	1.07670900
C	10.49980700	0.17299200	-0.38440200
H	11.39988700	0.23825800	0.23360400
H	10.56807600	-0.74232600	-0.98187300
H	10.50555500	1.02132600	-1.07704700

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The pyrolysis reaction: (Pathway A1) (Ketene product)

Basis set = 6-31G(d)

Nuclear repulsion energy= 1186.094607 Hartrees

E(RM062X) = -779.010725349 Hartrees
Formula: C16H32O2
Cartesian:

C	-7.74164700	0.48835000	-0.43173200
O	-7.80603400	1.60295400	-0.79165600
O	-5.72416900	2.70136800	0.96183200
H	-6.62724600	2.69512800	0.61261900
C	-7.66329600	-0.75783600	-0.03160300
H	-5.18121700	2.87920700	0.18229700
H	-8.60566600	-1.26339600	0.14823500
C	-6.33722100	-1.45038600	0.20392400
H	-6.29964600	-2.36740800	-0.39768300
H	-6.28327300	-1.76207400	1.25476100
C	-5.13574200	-0.56540700	-0.12373100
H	-5.17318400	-0.28935700	-1.18759800
H	-5.20738800	0.36797900	0.45080500
C	-3.80266800	-1.24623100	0.17433300
H	-3.76797000	-1.52557000	1.23627900
H	-3.72879100	-2.18316200	-0.39542100
C	-2.60385300	-0.35759800	-0.15101000
H	-2.68963300	0.58270100	0.41141900
H	-2.63203700	-0.08465600	-1.21540000
C	-1.26341200	-1.01692000	0.16575900
H	-1.23416000	-1.28568100	1.23087100
H	-1.18119000	-1.96092400	-0.39108400
C	-0.06506900	-0.12954600	-0.16409400
H	-0.15035500	0.81614800	0.38919900
H	-0.09165000	0.13586000	-1.23032500
C	1.27561600	-0.78507800	0.16012700
H	1.30236400	-1.04876400	1.22668600
H	1.36050200	-1.73196000	-0.39139000
C	2.47411800	0.10165800	-0.17091600
H	2.38739200	1.04961200	0.37837400
H	2.44915600	0.36313300	-1.23812600
C	3.81471700	-0.55169400	0.15805900
H	3.83949900	-0.81256200	1.22539400
H	3.90155100	-1.50002900	-0.39064600
C	5.01324100	0.33505200	-0.17288800
H	4.92531100	1.28396500	0.37458000
H	4.98953900	0.59468600	-1.24056400
C	6.35381500	-0.31696400	0.15888100
H	6.37712600	-0.57671100	1.22656000
H	6.44198300	-1.26587700	-0.38865500
C	7.55237700	0.56981600	-0.17113600
H	7.46450500	1.51915200	0.37591400
H	7.53024600	0.82955300	-1.23897000
C	8.89342700	-0.08131000	0.16158600
H	8.91338700	-0.34041000	1.22804200
H	8.97982900	-1.02865900	-0.38610400
C	10.08169300	0.81692700	-0.17231400

H	10.02822900	1.75758900	0.38603300
H	11.03288600	0.33530100	0.07183800
H	10.09494600	1.06560200	-1.23882500

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The pyrolysis reaction: (Pathway A) (Ketene + Palmitic acid)

Basis set = 6-31G(d)
Nuclear repulsion energy= 3170.790519 Hartrees
E(RM062X) = -1481.634011 Hartrees
Formula: C32H62O3
Cartesian:

C	-7.69814600	-2.39315300	1.22741800
O	-8.73867800	-2.69896700	0.77758600
C	-6.55999800	-2.06318300	1.78779600
H	-6.48317400	-2.32076200	2.84062900
C	-5.40039000	-1.38948000	1.08945500
H	-5.69412100	-1.11215100	0.07314100
H	-5.17723900	-0.45267800	1.61956100
C	-8.56346600	0.26802600	-0.69041800
O	-7.69344800	-0.53581500	-0.94383200
O	-9.67902200	-0.05401800	-0.02532200
H	-9.62522600	-1.00696400	0.19290400
C	-8.52737700	1.72479300	-1.09292300
H	-8.80058800	2.32664900	-0.21838700
H	-9.32653100	1.87510900	-1.82865800
C	-7.16062100	2.10997000	-1.64894500
H	-7.22589400	3.08378100	-2.14677300
H	-6.88143200	1.37532200	-2.41224900
C	-4.13862100	-2.25531200	1.05738800
H	-3.91554100	-2.62170000	2.06868600
H	-4.32560600	-3.14286300	0.44004700
C	-2.93286800	-1.48533300	0.52301600
H	-2.73307000	-0.62808900	1.18301000
H	-3.17540100	-1.06028700	-0.46239500
C	-1.66802400	-2.33418300	0.41697800
H	-1.47391600	-2.81765700	1.38470500
H	-1.82836400	-3.14580100	-0.30584300
C	-0.44424800	-1.51669000	0.01164800
H	-0.64111700	-1.01421800	-0.94672200
H	-0.28876100	-0.71463000	0.74876000
C	0.83665800	-2.34021400	-0.10070400
H	0.98255200	-2.91309700	0.82578200
H	0.73149900	-3.07972000	-0.90649000
C	2.06774700	-1.47329700	-0.35171000
H	2.17337100	-0.75578400	0.47610200
H	1.91226400	-0.86970000	-1.25806100
C	3.36505400	-2.26616500	-0.49096800
H	3.47828800	-2.93606000	0.37283100
H	3.30772800	-2.91333300	-1.37711700
C	4.59206200	-1.36332500	-0.59042800

H	4.66285200	-0.75435700	0.32349500
H	4.45592900	-0.65227200	-1.41879100
C	5.90267500	-2.12061300	-0.78943200
H	6.01066400	-2.87921700	-0.00165800
H	5.86813200	-2.66829300	-1.74143700
C	7.11928400	-1.19834100	-0.77212700
H	7.16801600	-0.68852000	0.20158500
H	6.98587700	-0.40608000	-1.52394800
C	8.44092100	-1.91766000	-1.02874700
H	8.57167700	-2.71703400	-0.28575400
H	8.40268200	-2.41361200	-2.00885700
C	9.64751200	-0.98204500	-0.98146900
H	9.68583600	-0.49389800	0.00150000
H	9.50930800	-0.17835700	-1.71709800
C	10.96496700	-1.70506800	-1.24948100
H	11.81640400	-1.01968100	-1.20982700
H	11.13385900	-2.49407400	-0.50897400
H	10.95765500	-2.17527800	-2.23857300
C	-6.07690400	2.15130000	-0.56888400
H	-6.20445700	3.05275800	0.04629600
H	-6.20043900	1.29276200	0.10339100
C	-4.66712500	2.11272700	-1.15193000
H	-4.54751100	2.91862700	-1.89013700
H	-4.54396300	1.16946300	-1.70360200
C	-3.57023400	2.22439800	-0.09598000
H	-3.65841600	3.18789000	0.42523300
H	-3.72333800	1.44736000	0.66692100
C	-2.16753700	2.08865900	-0.68327300
H	-2.08142700	1.11778400	-1.19292100
H	-2.02456400	2.85408500	-1.45940800
C	-1.05227100	2.20697400	0.35261500
H	-1.15208500	3.15797200	0.89450400
H	-1.16989100	1.41354100	1.10511500
C	0.34035100	2.12262800	-0.26869000
H	0.41659200	1.20460600	-0.86919600
H	0.47211100	2.95831400	-0.97054300
C	1.47193000	2.13841200	0.75585400
H	1.36341300	3.01203400	1.41398600
H	1.38291200	1.25530000	1.40600000
C	2.85580600	2.16145700	0.10939000
H	2.93063400	1.34423300	-0.62263400
H	2.97152200	3.09392800	-0.46084000
C	3.99798300	2.03366000	1.11394300
H	3.88904100	2.79783300	1.89651100
H	3.91966000	1.06268200	1.62552000
C	5.37788400	2.16232400	0.47156000
H	5.45666900	1.45954600	-0.37075700
H	5.48456600	3.16831300	0.04201000
C	6.52222500	1.89960800	1.44687800
H	6.41539500	2.55109000	2.32597800

H	6.44330100	0.86853100	1.82330100
C	7.90305200	2.10926700	0.82836100
H	7.98529700	1.50873100	-0.08752300
H	8.00324800	3.15714900	0.51763200
C	9.03412500	1.74168400	1.78467800
H	10.01621600	1.88993300	1.32561200
H	8.99176900	2.34975200	2.69477000
H	8.95989400	0.69054700	2.08698300

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The pyrolysis reaction in the presence of radicals generated from unsaturated acid (oliec acid): (Pathway B) (Reactant, R1B)

The first step is the formation of allylic radical.
Basis set = 6-31G(d)
Nuclear repulsion energy= 1356.1425074 Hartrees
E(RB3LYP) = -856.724481 Hartrees
Formula: C18H34O2
Cartesian:

C	8.43690400	-0.54199700	-0.11445500
C	7.13773600	0.24956500	0.04592400
C	5.89225400	-0.64417900	0.00753300
C	4.58230300	0.13831300	0.16695800
C	3.33164900	-0.74932500	0.13004200
C	2.02229000	0.03374200	0.28840900
C	0.76905700	-0.86200200	0.24965200
C	-0.51044800	-0.09632900	0.45210900
C	-1.50653600	-0.00327700	-0.43333700
C	-2.78622900	0.76205000	-0.23126600
C	-4.03943100	-0.13379600	-0.27054600
C	-5.34919200	0.64871300	-0.11269400
C	-6.60024900	-0.23856500	-0.14929300
C	-7.91112900	0.54271800	0.00925500
C	-9.16238300	-0.34403700	-0.02688500
C	-10.47353600	0.43653800	0.13178500
C	-11.71780300	-0.45668100	0.09459700
C	9.67474600	0.32748400	-0.07729300
O	9.70179600	1.53011300	0.06343500
O	10.80552900	-0.41178500	-0.22448000
H	11.54589100	0.22278900	-0.18860400
H	8.54029600	-1.30244000	0.67167100
H	8.44990600	-1.09997100	-1.06071300
H	7.17053000	0.80587300	0.99099600
H	7.07914200	1.00770500	-0.74496800
H	5.96073700	-1.40294700	0.80150800
H	5.86925600	-1.20069200	-0.94144200
H	4.60580000	0.69467100	1.11552300
H	4.51406100	0.89627400	-0.62709700
H	3.39988500	-1.50727700	0.92475800
H	3.30933300	-1.30626000	-0.81857500
H	2.04184400	0.58841500	1.23802700
H	1.94508800	0.79053100	-0.50445400

H	0.86599900	-1.62982300	1.03351300
H	0.73120100	-1.39965100	-0.70748700
H	-0.60309400	0.43285500	1.40392700
H	-1.41366400	-0.53260300	-1.38510500
H	-2.74881500	1.29980700	0.72580300
H	-2.88284400	1.52978300	-1.01520300
H	-3.96222600	-0.89067500	0.52233000
H	-4.05831000	-0.68852200	-1.22023400
H	-5.32716200	1.20614600	0.83563000
H	-5.41748500	1.40644900	-0.90760400
H	-6.53090800	-0.99632700	0.64525600
H	-6.62227300	-0.79581800	-1.09770500
H	-7.88880600	1.10018300	0.95758800
H	-7.98040100	1.30052000	-0.78545300
H	-9.09406900	-1.10204500	0.76784700
H	-9.18577500	-0.90172800	-0.97519800
H	-10.45070600	0.99319900	1.07956200
H	-10.54236700	1.19344900	-0.66259100
H	-11.69500200	-1.20184700	0.89944600
H	-12.63640400	0.12998600	0.21027200
H	-11.78729300	-1.00024100	-0.85582500

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The pyrolysis reaction in the presence of radicals generated from unsaturated acid (oliec acid): (Pathway B) (the 1st Transition State, TS1B)

The first step is the formation of allylic radical.
Basis set = 6-31G(d)
Nuclear repulsion energy= 1326.738177 Hartrees
E(RB3LYP) = -856.632121 Hartrees
Formula: C18H34O2
Cartesian:

C	-8.27477000	-0.74798700	-0.35274100
C	-7.06505000	-0.02007900	0.23623700
C	-5.78407800	-0.25002400	-0.57470800
C	-4.56352400	0.47487900	0.00686900
C	-3.27891500	0.24903300	-0.79915300
C	-2.05789900	0.97685200	-0.21604700
C	-0.80116200	0.77850300	-1.01037100
C	0.51843100	1.17016400	-0.48328400
C	1.39599200	0.34425100	0.10515300
C	2.73500500	0.74964100	0.65677700
C	3.91352200	0.02028400	-0.01670400
C	5.27634900	0.39467200	0.57906600
C	6.45420000	-0.32653800	-0.08899000
C	7.81834300	0.04634000	0.50599300
C	8.99662400	-0.67427300	-0.16157600
C	10.36100100	-0.30230500	0.43316300
C	11.53185900	-1.02647400	-0.23920700
C	-9.54620700	-0.52939700	0.43806400
O	-9.66005900	0.14018600	1.44084400

O	-10.59581900	-1.19090000	-0.11630900
H	-11.36463700	-0.99592900	0.45203700
H	-8.46679700	-0.43066900	-1.38682800
H	-8.09978800	-1.83105200	-0.40972300
H	-7.28465900	1.05334300	0.29320700
H	-6.91683000	-0.34999000	1.27204100
H	-5.94228200	0.08072400	-1.61217000
H	-5.57326900	-1.32852300	-0.62977500
H	-4.77438700	1.55310800	0.06184500
H	-4.40588000	0.14377800	1.04386200
H	-3.43478800	0.58238900	-1.83572500
H	-3.06303400	-0.82724000	-0.85412100
H	-2.29144200	2.05727500	-0.13905000
H	-1.88843800	0.65287800	0.82238500
H	-0.89962800	0.58811300	-2.07987800
H	1.98460700	0.93619900	-2.88843000
H	0.78972200	2.23191600	-0.55616500
H	1.14186600	-0.71420300	0.18978200
H	2.86456800	1.83537000	0.55321000
H	2.76383500	0.53360200	1.73660200
H	3.90371400	0.24565800	-1.09215500
H	3.76380700	-1.06602400	0.06875700
H	5.42253200	1.48199800	0.49666300
H	5.27604800	0.16988900	1.65621300
H	6.45379400	-0.10130000	-1.16577400
H	6.30746700	-1.41384000	-0.00716700
H	7.96479200	1.13375300	0.42439500
H	7.81840100	-0.17892300	1.58297600
H	8.99775200	-0.44895200	-1.23862700
H	8.85096000	-1.76195500	-0.08050400
H	10.50712400	0.78427400	0.35154100
H	10.36028800	-0.52798400	1.50915500
H	11.58024500	-0.79272500	-1.30999700
H	12.49075000	-0.73964400	0.20759800
H	11.43228000	-2.11484200	-0.14370100

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The pyrolysis reaction in the presence of radicals generated from unsaturated acid (oliec acid): (Pathway B) (the Product, P1B)

The first step is the formation of allylic radical.
Basis set = 6-31G(d)
Nuclear repulsion energy= 1325.547562 Hartrees
E(B3LYP) = -856.705886 Hartrees
Formula: C18H34O2
Cartesian:

C	8.30171000	0.33411500	0.40555200
C	7.05675400	-0.42498000	-0.05709500
C	5.79140900	0.44087900	-0.02718800
C	4.53580700	-0.30990400	-0.48895800
C	3.26627100	0.55030100	-0.45947700
C	2.00667000	-0.21154200	-0.92511300

C	0.77147500	0.63593300	-0.94252200
C	-0.36923800	0.38837300	-0.18711300
C	-1.51866400	1.17055000	-0.17367600
C	-2.73936200	0.87921700	0.64416900
C	-4.00034500	0.61923400	-0.20870600
C	-5.25650200	0.36430800	0.63372100
C	-6.51366600	0.10573800	-0.20681300
C	-7.77107800	-0.15044300	0.63424600
C	-9.02869100	-0.40914600	-0.20525400
C	-10.28635500	-0.66536700	0.63514400
C	-11.53739200	-0.92289400	-0.21102600
C	9.55800900	-0.50903200	0.38216700
O	9.63569800	-1.66963900	0.04481600
O	10.64004900	0.20048300	0.79726800
H	11.39638200	-0.41428100	0.75098200
H	8.48334000	1.22029600	-0.21779600
H	8.17761100	0.71883700	1.42707000
H	7.22538800	-0.80697200	-1.07167100
H	6.91982100	-1.31016200	0.57644500
H	5.93832000	1.32737700	-0.66219400
H	5.63177200	0.82210500	0.99248300
H	4.69446500	-0.68994900	-1.50894900
H	4.38988400	-1.19645800	0.14555700
H	3.40852800	1.43506400	-1.09687000
H	3.09907700	0.93043500	0.55770300
H	2.20123100	-0.60782700	-1.93564600
H	1.84942000	-1.08552100	-0.27844200
H	0.78115300	1.51015500	-1.59510800
H	-1.31133900	-1.48333900	-1.80108200
H	-0.35173900	-0.48336700	0.47112000
H	-1.55500200	2.04867000	-0.82007400
H	-2.55440900	0.01257900	1.29347400
H	-2.95024800	1.72837400	1.31544000
H	-3.81349800	-0.23970500	-0.86759700
H	-4.17171000	1.48077800	-0.87025000
H	-5.08052400	-0.49534400	1.29744400
H	-5.43178800	1.22640900	1.29464900
H	-6.33722500	-0.75568600	-0.86785700
H	-6.68969500	0.96545500	-0.87038200
H	-7.59470500	-1.01012200	1.29788600
H	-7.94715600	0.71112300	1.29556000
H	-8.85360000	-1.27096300	-0.86661800
H	-9.20603500	0.45024600	-0.86920900
H	-10.10960900	-1.52438500	1.29810700
H	-10.46190900	0.19594900	1.29545600
H	-11.40557000	-1.79998100	-0.85670300
H	-12.41713600	-1.10187600	0.41778000
H	-11.76035000	-0.06670600	-0.85972700

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The pyrolysis reaction in the presence of radicals generated from unsaturated acid (oliec acid): (Pathway B) (the Reactant, R2B)

The second step is the decarboxylation.
Basis set = 6-31G(d)
Nuclear repulsion energy= 3587.855740 Hartrees
E(UB3LYP) = -1636.158499 Hartrees
Formula: C34H66O4
Cartesian:
0 3

C	-8.73636700	5.50411000	-0.58495200
C	-8.10584400	4.36496700	-1.38808100
C	-7.72927500	3.16336600	-0.51306000
C	-7.09583500	2.01458500	-1.30852100
C	-6.70863400	0.81569500	-0.43449500
C	-6.08118600	-0.34235000	-1.23994500
C	-5.69187300	-1.51072900	-0.38678000
C	-4.42358700	-2.08265300	-0.35051800
C	-4.03917700	-3.15595400	0.44819100
C	-2.67946700	-3.78549400	0.43758800
C	-2.69249100	-5.25160000	-0.05051300
C	-1.30767400	-5.91021300	-0.01263100
C	-1.31315000	-7.36703100	-0.49364000
C	0.07018400	-8.02965000	-0.45426000
C	0.06535800	-9.48680700	-0.93364400
C	1.44777300	-10.15093400	-0.89349000
C	1.43369400	-11.60582800	-1.37344800
C	-9.10964900	6.69773600	-1.43666100
O	-8.94345500	6.80486600	-2.63174600
O	-9.67543000	7.68252500	-0.69118600
H	-9.88034100	8.40517800	-1.31397600
H	-9.64287900	5.17012600	-0.06211900
H	-8.05962200	5.85677600	0.20526800
H	-8.80293600	4.05192900	-2.17548300
H	-7.21699000	4.74255300	-1.90877300
H	-8.62464200	2.79297300	0.00785000
H	-7.03285400	3.48558700	0.27484900
H	-7.79423400	1.68573900	-2.09233700
H	-6.20367700	2.38658500	-1.83373800
H	-7.59880100	0.44311300	0.09223500
H	-6.00778400	1.13305900	0.34858800
H	-6.81075100	-0.66624900	-2.00117600
H	-5.20496100	0.02274600	-1.79382800
H	-6.46895000	-1.93662100	0.24984900
H	-2.43554100	0.91751300	-1.85502500
H	-3.66357400	-1.65302000	-1.00842000
H	-4.78663700	-3.60688200	1.10264400
H	-1.99955000	-3.19792400	-0.19438200
H	-2.25238800	-3.77041200	1.45374400
H	-3.09209600	-5.28389700	-1.07321900
H	-3.39110200	-5.83066600	0.57009400

H	-0.60983800	-5.32591400	-0.63066900
H	-0.91345900	-5.86730100	1.01359800
H	-1.70707400	-7.40900100	-1.51988800
H	-2.01268000	-7.95004200	0.12357400
H	0.76969200	-7.44662700	-1.07174000
H	0.46403100	-7.98657300	0.57214100
H	-0.32766300	-9.53068200	-1.96046900
H	-0.63448400	-10.07026500	-0.31676900
H	2.14698800	-9.56858000	-1.51042400
H	1.84025300	-10.10759200	0.13252200
H	1.07891100	-11.67824300	-2.40901100
H	2.43437800	-12.05101900	-1.33269500
H	0.76991400	-12.22134000	-0.75373600
C	-3.36917500	0.53533000	2.74163400
O	-3.34803500	1.29675900	3.67761700
O	-4.51836500	-0.11396500	2.41740500
H	-4.38969900	-0.69465700	1.64270900
C	-2.16969300	0.22871100	1.85174100
H	-2.44165100	0.47425500	0.81389800
H	-2.00137200	-0.85823300	1.86256500
C	-0.90255800	0.97810300	2.26723000
H	-1.11016400	2.05504400	2.26580100
H	-0.66253000	0.72273000	3.30659000
C	0.29520000	0.67204900	1.36003500
H	0.49529100	-0.41016400	1.36750500
H	0.04169900	0.92548300	0.31935700
C	1.56878000	1.42431900	1.76717700
H	1.36801700	2.50570800	1.75953200
H	1.82184400	1.17098300	2.80715400
C	2.77243900	1.12514200	0.86433900
H	2.51755400	1.37676700	-0.17607600
H	2.97368500	0.04340900	0.87355400
C	4.04489700	1.88016400	1.27005500
H	4.29972800	1.62883600	2.31036000
H	3.84315500	2.96162200	1.26100400
C	5.24928300	1.58234700	0.36753500
H	4.99366000	1.83238900	-0.67303400
H	5.45200500	0.50093700	0.37770300
C	6.52086600	2.33952100	0.77199600
H	6.77650600	2.08966700	1.81252700
H	6.31779500	3.42078600	0.76188000
C	7.72549100	2.04246000	-0.13047200
H	7.46934300	2.29135800	-1.17117200
H	7.92935200	0.96128500	-0.11954400
C	8.99641500	2.80123500	0.27305200
H	9.25259500	2.55246800	1.31373700
H	8.79233200	3.88232600	0.26212400
C	10.20113600	2.50461600	-0.62942700
H	9.94464000	2.75274700	-1.67021300
H	10.40575600	1.42360100	-0.61795800

C	11.47164500	3.26442500	-0.22656900
H	11.72814500	3.01637200	0.81424700
H	11.26688400	4.34542000	-0.23807000
C	12.67650300	2.96829900	-1.12873300
H	12.42093100	3.21616300	-2.16995300
H	12.88261500	1.88742900	-1.11728400
C	13.94697900	3.72840200	-0.72655500
H	14.20301300	3.48035100	0.31344300
H	13.74149400	4.80835400	-0.73867000
C	15.14505100	3.42685400	-1.63270800
H	14.93219800	3.69731900	-2.67440800
H	16.03530000	3.98431400	-1.31952100
H	15.39714600	2.35927900	-1.61440400

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The pyrolysis reaction in the presence of radicals generated from unsaturated acid (oliec acid): (Pathway B) (Transition State, TS2B)

The second step is the decarboxylation.
Basis set = 6-31G(d)
Nuclear repulsion energy= 3612.085630 Hartrees
E(UB3LYP) = -1635.944552 Hartrees
Formula: C34H66O4
Cartesian:
0 3

C	-2.33513000	8.44637000	-0.38828100
C	-3.12108200	7.38010300	-1.15348000
C	-3.50183700	6.18228200	-0.27497300
C	-4.29077600	5.10694700	-1.03310900
C	-4.67126000	3.90508300	-0.15997700
C	-5.46187200	2.82442300	-0.93049600
C	-5.87266400	1.66760100	-0.07197400
C	-5.44521400	0.35565500	-0.25534800
C	-5.79299800	-0.73108500	0.54197100
C	-5.34702800	-2.14140500	0.30345700
C	-6.51437900	-3.10678900	0.00012700
C	-6.05793000	-4.55743300	-0.20009900
C	-7.21158200	-5.52389300	-0.49812100
C	-6.75686400	-6.97512700	-0.70121900
C	-7.90959400	-7.94309400	-0.99697900
C	-7.45562500	-9.39423500	-1.20128600
C	-8.61296600	-10.35420000	-1.49515900
C	-1.95077500	9.63268800	-1.24536800
O	-2.20402100	9.77890100	-2.42080400
O	-1.26092800	10.55930100	-0.53037300
H	-1.05563900	11.28044800	-1.15479800
H	-2.90731500	8.82543000	0.46939700
H	-1.41243600	8.03133300	0.03976300
H	-4.02443100	7.83560700	-1.57808600
H	-2.52591600	7.04178100	-2.01083700
H	-4.09524600	6.52997000	0.58362400

H	-2.59144100	5.73313400	0.14872300
H	-5.20300900	5.55456900	-1.45444900
H	-3.69790600	4.76038100	-1.89239200
H	-5.26787300	4.24684900	0.69754200
H	-3.76460200	3.44989200	0.26162000
H	-6.35683200	3.29794200	-1.36585800
H	-4.85977200	2.46568000	-1.77625000
H	-6.54025000	1.88348100	0.76345200
H	-2.45624600	0.83338100	0.80735100
H	-4.78193200	0.16176700	-1.10161000
H	-6.46276800	-0.56085700	1.38611600
H	-4.62627100	-2.17027500	-0.52528200
H	-4.81515300	-2.51961200	1.19181700
H	-7.04410200	-2.75672300	-0.89629900
H	-7.24164600	-3.06130800	0.82331900
H	-5.32792300	-4.59856700	-1.02218800
H	-5.52205100	-4.89666800	0.69888200
H	-7.74857300	-5.18255400	-1.39550400
H	-7.94044300	-5.48343200	0.32488200
H	-6.02873700	-7.01527100	-1.52509500
H	-6.21821000	-7.31552900	0.19569900
H	-8.44931100	-7.60303700	-1.89355700
H	-8.63765900	-7.90426600	-0.17286600
H	-6.72910600	-9.43338700	-2.02548000
H	-6.91646500	-9.73411400	-0.30551200
H	-9.15024100	-10.06057600	-2.40546600
H	-8.25626400	-11.38094600	-1.63590900
H	-9.33875400	-10.36364300	-0.67257100
C	-2.63221500	1.00342400	2.85921600
O	-2.08114100	1.28349100	3.88256000
O	-3.89519600	1.29712500	2.56386700
H	-4.09510100	1.01769100	1.64201600
C	-1.69354100	0.08769400	1.57602000
H	-1.95693500	-0.74975600	0.88630600
H	-1.45441700	-0.57949500	2.47700200
C	-0.30824000	0.69148600	1.24276500
H	-0.35553200	1.21318700	0.27781200
H	-0.07925500	1.45113600	2.00011600
C	0.81663200	-0.35133400	1.21324600
H	0.86087500	-0.86494400	2.18437500
H	0.58034300	-1.12454100	0.46682200
C	2.19014400	0.25471500	0.89662000
H	2.14402000	0.77630200	-0.07101900
H	2.42652600	1.02463400	1.64567700
C	3.32130500	-0.78114900	0.85904600
H	3.08498900	-1.54959600	0.10785000
H	3.36543200	-1.30536400	1.82519300
C	4.69615000	-0.17527600	0.54846800
H	4.93413800	0.58935100	1.30280400
H	4.65033200	0.35410000	-0.41500300

C	5.82697300	-1.21114100	0.50311100
H	5.59007300	-1.97392700	-0.25363800
H	5.87091500	-1.74298100	1.46523300
C	7.20249400	-0.60449600	0.19696700
H	7.44107000	0.15507500	0.95631200
H	7.15729700	-0.06864600	-0.76294500
C	8.33267700	-1.64075300	0.14495600
H	8.09489900	-2.39890700	-0.61614600
H	8.37668200	-2.17839700	1.10388100
C	9.70855000	-1.03343400	-0.15825500
H	9.94768200	-0.27770700	0.60477500
H	9.66358000	-0.49283600	-1.11551000
C	10.83815400	-2.07004600	-0.21540200
H	10.59949700	-2.82485400	-0.97953300
H	10.88245900	-2.61177800	0.74121300
C	12.21421100	-1.46231300	-0.51691200
H	12.45374800	-0.70903500	0.24846400
H	12.16925500	-0.91869800	-1.47248500
C	13.34356400	-2.49874500	-0.57745500
H	13.10531800	-3.25192400	-1.34351400
H	13.38932100	-3.04323700	0.37769200
C	14.71982200	-1.89122100	-0.87817000
H	14.95875800	-1.13979000	-0.11205700
H	14.67439900	-1.34715700	-1.83243700
C	15.84141000	-2.93329100	-0.93796900
H	15.64840300	-3.67897600	-1.71918500
H	16.81012000	-2.46818400	-1.15402800
H	15.93481500	-3.47023600	0.01416600

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The pyrolysis reaction in the presence of radicals generated from unsaturated acid (oliec acid): (Pathway B) (the Product, P2B)

The second step is the decarboxylation.
Basis set = 6-31G(d)
Nuclear repulsion energy= 3709.291978 Hartrees
E(UB3LYP) = -1636.215306 Hartrees
Formula: C34H66O4
Cartesian:
0 3

C	13.03974600	-1.10688600	-0.25962700
C	11.69439900	-1.46054800	0.37682800
C	10.51518800	-0.75322900	-0.30168700
C	9.16102200	-1.09820800	0.33142000
C	7.97688000	-0.39517200	-0.34404300
C	6.62494600	-0.73974700	0.29215300
C	5.44574000	-0.03157700	-0.39228700
C	4.12454000	-0.24735100	0.24208300
C	2.93002100	-0.14155200	-0.41033000
C	1.58641100	-0.27416000	0.22019800
C	0.68905800	-1.32954800	-0.46048200

C	-0.72100300	-1.37949400	0.14130000
C	-1.63025700	-2.42019600	-0.52459100
C	-3.04464000	-2.46145700	0.06881800
C	-3.95740100	-3.50056200	-0.59467000
C	-5.37291500	-3.53978100	-0.00438100
C	-6.27698700	-4.58197000	-0.67052300
C	14.21110900	-1.80463500	0.39684800
O	14.15351200	-2.58107000	1.32465600
O	15.38723400	-1.45676500	-0.18745300
H	16.08022000	-1.94778600	0.29295600
H	13.05539300	-1.36356400	-1.32774800
H	13.22904600	-0.02564900	-0.21846600
H	11.55297200	-2.54777700	0.33639600
H	11.72271400	-1.20237300	1.44280300
H	10.49430300	-1.01692000	-1.36970600
H	10.66704100	0.33557600	-0.26151600
H	9.00967200	-2.18709200	0.29303400
H	9.18184000	-0.83193500	1.39835200
H	7.95504700	-0.66301100	-1.41075500
H	8.12611100	0.69330300	-0.30675400
H	6.46841800	-1.82746300	0.25734700
H	6.64145300	-0.46506200	1.35651800
H	5.40380100	-0.27498500	-1.46307400
H	2.10567200	5.75094600	-0.16603300
H	4.10687200	-0.41044000	1.32092000
H	2.94561000	0.02419000	-1.48775500
H	1.68858900	-0.49262100	1.29067300
H	1.09695300	0.70949200	0.14411300
H	1.16134800	-2.31828100	-0.37962800
H	0.62036900	-1.10686800	-1.53475600
H	-0.64994700	-1.59331300	1.21785800
H	-1.18302900	-0.38473900	0.05824200
H	-1.16973900	-3.41544200	-0.43670400
H	-1.69483500	-2.20927600	-1.60226400
H	-2.98011300	-2.67023100	1.14707200
H	-3.50376700	-1.46548700	-0.02041300
H	-3.49993300	-4.49727800	-0.50425500
H	-4.02081300	-3.29320500	-1.67336500
H	-5.30988300	-3.74499800	1.07382200
H	-5.83140400	-2.54467600	-0.09786000
H	-5.86338600	-5.59238500	-0.56292800
H	-7.27965400	-4.58393700	-0.22799900
H	-6.38729700	-4.38308200	-1.74368800
C	3.86064800	3.20876300	-0.26902500
O	2.94416800	2.36509900	-0.03973300
O	5.05313100	2.99587500	-0.51564900
H	5.61078300	1.07278200	-0.36447500
C	1.07156600	5.85901400	0.17940700
H	0.68916900	6.82338500	-0.17858700
H	1.09227600	5.89830400	1.27591200

C	0.20628500	4.69487700	-0.31301500
H	0.19707400	4.68675500	-1.41272200
H	0.67451500	3.74905300	-0.00883400
C	-1.23730100	4.74193000	0.20336000
H	-1.22785800	4.75804900	1.30372700
H	-1.70730900	5.68701700	-0.10850300
C	-2.09677500	3.56543800	-0.27721500
H	-2.11125300	3.55176400	-1.37738400
H	-1.61969200	2.62194100	0.03016100
C	-3.53786000	3.59552800	0.24782800
H	-4.01798500	4.53552300	-0.06256400
H	-3.52305000	3.61250600	1.34783500
C	-4.38928300	2.41133900	-0.22835900
H	-3.90577800	1.47120200	0.07892600
H	-4.40754200	2.39626700	-1.32838600
C	-5.82875200	2.43439000	0.30168300
H	-6.31376300	3.37270200	-0.00617200
H	-5.81018500	2.45029800	1.40162200
C	-6.67674500	1.24722000	-0.17306800
H	-6.18918700	0.30874400	0.13233200
H	-6.69794700	1.23301700	-1.27302200
C	-8.11483300	1.26570600	0.36090100
H	-8.60302100	2.20325400	0.05567300
H	-8.09327900	1.28018300	1.46081900
C	-8.96096300	0.07696000	-0.11313700
H	-8.47138700	-0.86074500	0.19036700
H	-8.98415100	0.06363800	-1.21306500
C	-10.39824800	0.09353500	0.42325400
H	-10.88789300	1.03082700	0.11952400
H	-10.37490500	0.10729700	1.52316200
C	-11.24419200	-1.09565300	-0.05002200
H	-10.75433500	-2.03300600	0.25350900
H	-11.26776200	-1.10928800	-1.14997400
C	-12.68122600	-1.07920200	0.48656100
H	-13.17216300	-0.14237500	0.18295500
H	-12.65862600	-1.06571500	1.58663900
C	-13.52757000	-2.26832000	0.01400000
H	-13.03765200	-3.20448500	0.31781800
H	-13.55111400	-2.28150900	-1.08507200
C	-14.96089800	-2.24381400	0.55473800
H	-15.48851400	-1.33552600	0.23818000
H	-15.53851900	-3.10497000	0.19953100
H	-14.97121700	-2.26547300	1.65155800

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The pyrolysis reaction: (Pathway A2) (Reactant, RA2)

Basis set = 6-31+G(d)

Nuclear repulsion energy= 3032.6158347723Hartrees

E(UB3LYP) = -1482.51423738

Formula C32H62O3

Charge = 0 Multiplicity = 1

C	-1.17964	5.86104	0.04065
O	-1.60987	6.95935	0.27263
C	-1.9416	4.79161	-0.71656
C	-3.07725	4.19967	0.14511
H	-1.27764	3.99943	-1.0716
H	-2.37451	5.29218	-1.58975
C	-3.95169	3.213	-0.63756
H	-2.63848	3.69142	1.01304
H	-3.69228	5.02343	0.52858
H	-4.38256	3.72367	-1.5113
H	-3.32197	2.40376	-1.03502
O	0.09971	5.56316	0.50732
C	0.59988	4.27338	0.48549
C	1.52938	3.87981	-0.38566
H	1.80813	4.59586	-1.15396
C	2.22089	2.54538	-0.36268
C	3.75384	2.66891	-0.26976
H	1.96952	1.98517	-1.27669
H	1.84474	1.95077	0.47719
H	4.11998	3.29006	-1.10037
H	4.01451	3.20793	0.65145
C	4.46819	1.3119	-0.2946
H	4.20113	0.77776	-1.21878
H	4.09501	0.69038	0.53293
C	5.9952	1.42259	-0.19617
H	6.36828	2.04496	-1.02314
H	6.26124	1.95642	0.72822
C	6.71043	0.06549	-0.22096
H	6.44611	-0.46727	-1.14663
H	6.3348	-0.55759	0.60439
C	8.23731	0.17459	-0.11799
H	8.61322	0.79803	-0.94294
H	8.50127	0.70699	0.80795
C	8.95217	-1.18266	-0.14275
H	8.68964	-1.71423	-1.06962
H	8.57449	-1.80667	0.68099
C	10.47889	-1.07453	-0.0364
H	10.85683	-0.45027	-0.85982
H	10.74123	-0.54333	0.89072
C	11.19332	-2.432	-0.06132
H	10.932	-2.96262	-0.98908
H	10.81418	-3.05667	0.76126
C	12.71991	-2.32451	0.04735
H	13.09921	-1.69964	-0.77498
H	12.98114	-1.79421	0.9753
C	13.43408	-3.68211	0.02221
H	13.17342	-4.21208	-0.90614
H	13.0541	-4.30722	0.84409
C	14.96046	-3.57537	0.13213

H	15.22214	-3.04601	1.06066
H	15.34157	-2.95052	-0.68957
C	15.67492	-4.93275	0.10685
H	15.41448	-5.46141	-0.82126
H	15.2947	-5.55703	0.92806
C	17.19864	-4.81678	0.21754
H	17.49175	-4.32348	1.1526
H	17.67859	-5.80197	0.1965
H	17.61245	-4.22704	-0.60985
C	-5.08102	2.60952	0.20767
H	-5.7064	3.42036	0.60932
H	-4.64734	2.09914	1.08027
C	-5.96464	1.62426	-0.56845
H	-6.39925	2.13558	-1.44021
H	-5.33803	0.81536	-0.97267
C	-7.09194	1.01738	0.27693
H	-7.71701	1.8267	0.68275
H	-6.65664	0.50534	1.14802
C	-7.97805	0.03345	-0.49798
H	-7.35274	-0.77504	-0.90526
H	-8.41449	0.54601	-1.3682
C	-9.10384	-0.57491	0.34838
H	-8.66704	-1.08822	1.21802
H	-9.72819	0.23376	0.75674
C	-9.99162	-1.55772	-0.42607
H	-9.36721	-2.36591	-0.83535
H	-10.42925	-1.04407	-1.29508
C	-11.11636	-2.16685	0.42112
H	-10.67852	-2.68115	1.28966
H	-11.74007	-1.35854	0.8312
C	-12.00534	-3.1487	-0.35317
H	-11.38164	-3.95677	-0.76379
H	-12.44366	-2.6342	-1.22133
C	-13.12951	-3.75823	0.49448
H	-12.69105	-4.27321	1.36235
H	-13.75277	-2.95006	0.90562
C	-14.01936	-4.73936	-0.27937
H	-13.39698	-5.54821	-0.69083
H	-14.45887	-4.22501	-1.1472
C	-15.1434	-5.34922	0.56808
H	-14.70445	-5.86397	1.43472
H	-15.76576	-4.54135	0.97879
C	-16.02721	-6.32749	-0.21249
H	-15.43899	-7.16571	-0.60618
H	-16.81918	-6.74491	0.41992
H	-16.5082	-5.83311	-1.06561
O	0.07421	3.4706	1.45961
H	-0.12137	4.03061	2.23021

****

The pyrolysis reaction: (Pathway A2) (TS2A2)
Basis set = 6-31+G(d)
Nuclear repulsion energy= 3017.7256284840 Hartrees
E(UB3LYP) = -1482.43148721
Formula C32H62O3

Charge = 0 Multiplicity = 1

C	-0.08844	1.26985	0.63514
O	-0.1138	1.27294	1.85679
C	-1.32438	0.98761	-0.20578
C	-2.61802	0.88397	0.60362
H	-1.13472	0.05122	-0.75573
H	-1.39891	1.76197	-0.98218
C	-3.84092	0.56417	-0.26489
H	-2.49611	0.11757	1.37873
H	-2.77995	1.82695	1.1416
H	-3.95125	1.33538	-1.04181
H	-3.67297	-0.38259	-0.8004
O	0.2082	3.71105	-1.45758
C	1.01983	3.47697	-0.63479
C	1.19739	1.55218	-0.10133
H	1.19081	1.21349	-1.13952
C	2.45333	0.94274	0.62427
C	3.75489	1.07201	-0.17547
H	2.2181	-0.11698	0.79462
H	2.5653	1.37608	1.62575
H	3.62398	0.60138	-1.16055
H	3.97238	2.13178	-0.36936
C	4.95301	0.43319	0.53991
H	4.73731	-0.62773	0.734
H	5.07869	0.90361	1.52586
C	6.26329	0.54999	-0.24959
H	6.1367	0.07946	-1.23592
H	6.47536	1.61157	-0.44455
C	7.46406	-0.08405	0.46444
H	7.25242	-1.14626	0.65753
H	7.5874	0.38465	1.452
C	8.77658	0.03675	-0.32071
H	8.65351	-0.43198	-1.30846
H	8.98704	1.09917	-0.51392
C	9.97808	-0.59548	0.39377
H	9.76848	-1.65846	0.5852
H	10.09907	-0.12818	1.38242
C	11.29186	-0.47128	-0.38874
H	11.17122	-0.93867	-1.37745
H	11.50083	0.59181	-0.58023
C	12.49361	-1.10238	0.32632
H	12.28531	-2.16586	0.51655
H	12.61293	-0.63596	1.31563
C	13.80814	-0.97582	-0.45455

H	13.68907	-1.44233	-1.44387
H	14.0161	0.08771	-0.64481
C	15.01	-1.60626	0.2609
H	14.80239	-2.67002	0.45049
H	15.12836	-1.14024	1.25057
C	16.32497	-1.47863	-0.51872
H	16.53356	-0.41498	-0.70846
H	16.20785	-1.94486	-1.50856
C	17.52708	-2.10863	0.19658
H	17.31929	-3.17157	0.38547
H	17.64466	-1.64252	1.1853
C	18.83598	-1.97638	-0.58872
H	19.08906	-0.92321	-0.76295
H	19.67404	-2.43548	-0.05182
H	18.76131	-2.46381	-1.56873
C	-5.14415	0.46576	0.53869
H	-5.31166	1.41228	1.07346
H	-5.03349	-0.30515	1.31555
C	-6.37268	0.14587	-0.32265
H	-6.48152	0.91666	-1.10018
H	-6.20528	-0.80136	-0.85692
C	-7.67611	0.05016	0.48093
H	-7.84267	0.99709	1.01571
H	-7.5675	-0.72094	1.25816
C	-8.90575	-0.26802	-0.37962
H	-8.73962	-1.21533	-0.91407
H	-9.01377	0.50291	-1.15715
C	-10.20925	-0.36219	0.42404
H	-10.10152	-1.13348	1.20125
H	-10.37476	0.58491	0.95895
C	-11.43941	-0.67896	-0.4363
H	-11.27425	-1.62632	-0.97094
H	-11.54674	0.09219	-1.21372
C	-12.74298	-0.77203	0.36738
H	-12.63591	-1.54346	1.14455
H	-12.90773	0.17519	0.90234
C	-13.97339	-1.08778	-0.49298
H	-13.80887	-2.03518	-1.02774
H	-14.08016	-0.31647	-1.27031
C	-15.27707	-1.1801	0.31057
H	-15.17046	-1.9516	1.08777
H	-15.44135	-0.23275	0.84552
C	-16.50766	-1.4952	-0.54946
H	-16.34462	-2.44288	-1.08444
H	-16.61521	-0.72395	-1.32694
C	-17.8116	-1.58715	0.25359
H	-17.70478	-2.35826	1.02991
H	-17.97507	-0.64019	0.78765
C	-19.03524	-1.90182	-0.6131
H	-18.91683	-2.86066	-1.13292

H	-19.94913	-1.96055	-0.01081
H	-19.18898	-1.12964	-1.37709
O	1.89857	3.97851	0.1207
H	1.8291	2.7304	0.34411

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The pyrolysis reaction: (Pathway A2) (Intermediate 2, I2A2)

Basis set = 6-31+G(d)
Nuclear repulsion energy= 3052.6423025845 Hartrees
E(UB3LYP) = -1482.55143636
Formula C32H62O3
Charge = 0 Multiplicity = 1

C	-0.11066	3.68477	0.2272
O	-0.33761	4.23725	1.29942
C	-1.16213	2.86076	-0.48411
C	-2.45045	2.64336	0.31163
H	-0.70558	1.90309	-0.77728
H	-1.37051	3.37211	-1.43794
C	-3.4919	1.82336	-0.46016
H	-2.20836	2.14339	1.25826
H	-2.86933	3.61863	0.5874
H	-3.72719	2.32961	-1.40828
H	-3.06135	0.84896	-0.73579
O	2.60542	5.59817	-1.23269
C	1.91613	5.16713	-0.33834
C	1.26673	3.77292	-0.42038
H	1.19859	3.52313	-1.48331
C	2.19171	2.72298	0.27649
C	3.55107	2.54172	-0.41066
H	1.66556	1.75831	0.29782
H	2.32888	3.02525	1.32232
H	3.3894	2.23283	-1.45313
H	4.07431	3.50378	-0.45859
C	4.43211	1.50606	0.30092
H	3.90265	0.54251	0.34779
H	4.58974	1.81756	1.344
C	5.79305	1.30407	-0.37832
H	5.63512	0.99378	-1.42181
H	6.32036	2.26789	-0.4253
C	6.6813	0.27235	0.3289
H	6.15196	-0.69111	0.3769
H	6.83906	0.58356	1.37227
C	8.04206	0.06903	-0.34995
H	7.88412	-0.24069	-1.39379
H	8.57132	1.03227	-0.39701
C	8.93091	-0.96344	0.35555
H	8.40114	-1.92667	0.40277
H	9.08881	-0.65357	1.39936
C	10.29164	-1.16706	-0.32325

H	10.13366	-1.47585	-1.36739
H	10.82163	-0.20406	-0.36963
C	11.18023	-2.20048	0.38122
H	10.65004	-3.16349	0.42761
H	11.33819	-1.89167	1.42536
C	12.54096	-2.4042	-0.29755
H	12.38298	-2.71236	-1.34189
H	13.07134	-1.44136	-0.34338
C	13.42926	-3.43825	0.40632
H	12.89875	-4.40114	0.45213
H	13.58719	-3.13007	1.45069
C	14.78997	-3.64228	-0.272
H	15.3216	-2.67993	-0.31766
H	14.6331	-3.95068	-1.31658
C	15.67838	-4.67649	0.43137
H	15.14775	-5.63832	0.4764
H	15.83585	-4.36817	1.47484
C	17.03515	-4.87384	-0.2525
H	17.60458	-3.93656	-0.28126
H	17.64498	-5.6176	0.27317
H	16.91138	-5.21605	-1.28747
C	-4.78833	1.59848	0.32878
H	-5.21926	2.57273	0.60232
H	-4.55227	1.09434	1.27748
C	-5.83401	0.77695	-0.43619
H	-6.06881	1.2814	-1.38531
H	-5.40136	-0.19696	-0.70979
C	-7.13104	0.55125	0.35156
H	-7.56441	1.52513	0.62366
H	-6.89579	0.04866	1.30153
C	-8.17592	-0.2727	-0.41205
H	-7.74198	-1.24653	-0.68396
H	-8.41067	0.22978	-1.36227
C	-9.47335	-0.49886	0.37491
H	-9.23833	-1.00002	1.32576
H	-9.90798	0.47492	0.64565
C	-10.51725	-1.32473	-0.38799
H	-10.08232	-2.29849	-0.65855
H	-10.75201	-0.8237	-1.33899
C	-11.81492	-1.55116	0.39852
H	-11.58	-2.0513	1.34995
H	-12.25038	-0.57744	0.66825
C	-12.85807	-2.37837	-0.36395
H	-12.42245	-3.35209	-0.63355
H	-13.09286	-1.87833	-1.31547
C	-14.15587	-2.60497	0.42228
H	-13.92096	-3.1045	1.37407
H	-14.59179	-1.63123	0.6914
C	-15.19874	-3.43284	-0.33952
H	-14.76375	-4.40711	-0.6087

H	-15.43461	-2.93385	-1.29148
C	-16.49668	-3.6597	0.44627
H	-16.26133	-4.15879	1.39717
H	-16.93197	-2.68644	0.71453
C	-17.53226	-4.48744	-0.32174
H	-17.13858	-5.47995	-0.57375
H	-18.44632	-4.63145	0.26573
H	-17.81429	-3.99649	-1.26143
O	1.73345	5.83779	0.81031
H	1.03825	5.37438	1.33823

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The pyrolysis reaction: (Pathway A2) (Product, PA2)

Basis set = 6-31+G(d)
Nuclear repulsion energy= 3020.2941717892 Hartrees
E(UB3LYP) = -1482.56525149
Formula C32H62O3
Charge = 0 Multiplicity = 1

C	-0.02204	-0.29424	-0.33876
O	-0.01791	0.57518	-1.1861
C	1.26903	-0.81592	0.26551
C	2.51767	-0.20188	-0.35478
H	1.27904	-1.91126	0.17383
H	1.22844	-0.61301	1.34556
C	3.80538	-0.73321	0.26974
H	2.51545	-0.39459	-1.43405
H	2.4748	0.88975	-0.25169
H	3.79609	-0.5413	1.35208
H	3.84577	-1.82553	0.15373
O	0.7179	3.3565	-0.10572
C	0.23905	2.64051	0.67129
C	-1.31412	-0.88908	0.18728
H	-1.32681	-1.95616	-0.07953
C	-2.55834	-0.18352	-0.33519
C	-3.84993	-0.80737	0.18728
H	-2.54765	-0.19851	-1.431
H	-2.51226	0.87378	-0.04671
H	-3.88963	-1.86721	-0.10187
H	-3.84831	-0.78977	1.28625
C	-5.10095	-0.09781	-0.32636
H	-5.10366	-0.11699	-1.425
H	-5.06008	0.96198	-0.03896
C	-6.39773	-0.71355	0.19449
H	-6.43837	-1.77374	-0.0924
H	-6.39397	-0.69378	1.29338
C	-7.64824	-0.00302	-0.31907
H	-7.6531	-0.02461	-1.41783
H	-7.60605	1.05761	-0.03431
C	-8.94582	-0.61514	0.20426
H	-8.98834	-1.67589	-0.0802

H	-8.94082	-0.59309	1.30309
C	-10.19583	0.09618	-0.30944
H	-10.20173	0.07268	-1.40819
H	-10.15204	1.15729	-0.02659
C	-11.49385	-0.51325	0.21595
H	-11.53803	-1.57438	-0.06682
H	-11.48781	-0.48957	1.31474
C	-12.74344	0.19887	-0.29765
H	-12.75018	0.17413	-1.39639
H	-12.69832	1.26027	-0.01604
C	-14.04173	-0.40861	0.22933
H	-14.08719	-1.46998	-0.05233
H	-14.03483	-0.38385	1.32807
C	-15.29107	0.30417	-0.28401
H	-15.29839	0.27868	-1.38276
H	-15.2449	1.36574	-0.00313
C	-16.58955	-0.30174	0.24387
H	-16.58288	-0.27648	1.34276
H	-16.63671	-1.36343	-0.03687
C	-17.83928	0.41118	-0.26902
H	-17.84456	0.38447	-1.36635
H	-17.79023	1.47114	0.01195
C	-19.12897	-0.20466	0.26737
H	-19.15515	-0.16316	1.36147
H	-20.01293	0.31772	-0.10958
H	-19.20994	-1.2568	-0.02576
C	5.06061	-0.1144	-0.34163
H	5.02283	0.97704	-0.22056
H	5.06694	-0.30178	-1.42428
C	6.3531	-0.64804	0.2722
H	6.34453	-0.46453	1.35583
H	6.39177	-1.73928	0.14691
C	7.60802	-0.02507	-0.33557
H	7.57123	1.06565	-0.20635
H	7.61418	-0.20447	-1.41979
C	8.9015	-0.56283	0.27273
H	8.93935	-1.65328	0.14068
H	8.89437	-0.38613	1.35747
C	10.15602	0.06316	-0.33277
H	10.16138	-0.11062	-1.41796
H	10.11952	1.15325	-0.19789
C	11.45007	-0.47766	0.27162
H	11.4873	-1.56755	0.13492
H	11.44419	-0.30561	1.35711
C	12.70423	0.15031	-0.33256
H	12.70894	-0.01988	-1.41834
H	12.66787	1.23997	-0.19405
C	13.99865	-0.39248	0.26927
H	14.03542	-1.48201	0.12975
H	13.99369	-0.22325	1.35521

C	15.25259	0.2366	-0.33423
H	15.25684	0.06834	-1.42034
H	15.21617	1.32605	-0.19379
C	16.54729	-0.30688	0.26595
H	16.58465	-1.39641	0.12536
H	16.54378	-0.13911	1.35227
C	17.80159	0.32241	-0.33721
H	17.8033	0.15391	-1.42186
H	17.76265	1.41021	-0.19567
C	19.08755	-0.23042	0.27188
H	19.15834	-1.31237	0.11752
H	19.97481	0.23062	-0.17152
H	19.11771	-0.04761	1.35129
O	-0.23219	1.94089	1.47681
H	-1.27756	-0.85957	1.28499