

Unimolecular Reaction Chemistry of a Charge-Tagged *beta*-Hydroxyperoxyl Radical

Electronic Supplementary Information

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SUMMARY

This Electronic Supplementary Information is 23 pages and contains the mass spectroscopy of the photodissociation and collision induced dissociation to produce the target radical anion. Master equation simulation with and without pre-reaction complex using M06-2X and G3SX barrier heights at 307 K and 2.5 mTorr He. Optimized geometries, vibrational frequencies and moments of inertia of the wells and transition states at M06-2X level of theory. Reaction schemes of the isotope labeling experiments. This information is available free of charge via the Internet at <http://pubs.acs.org>.

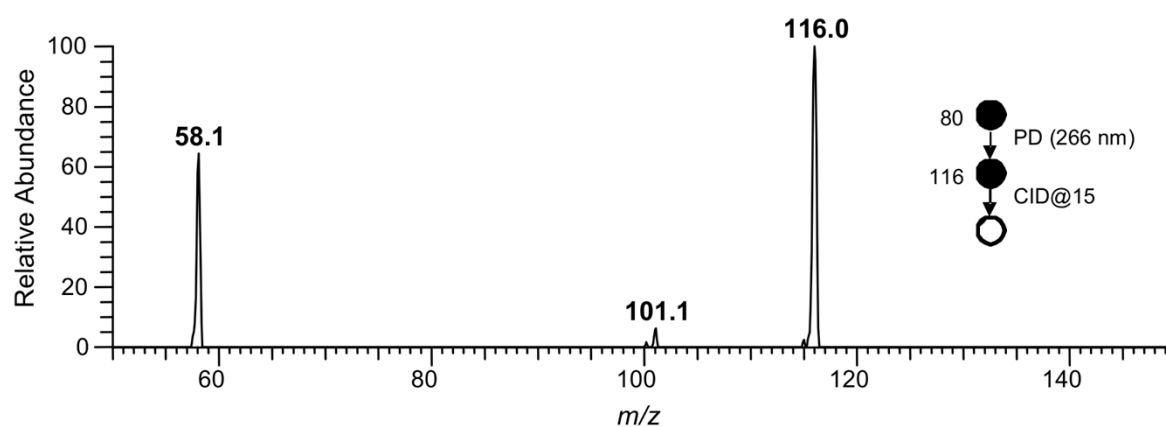


Figure S1. Mass spectroscopy of the photodissociation of the isolated dianion (m/z 80) producing the radical anion (m/z 116), followed by the collision induced dissociation.

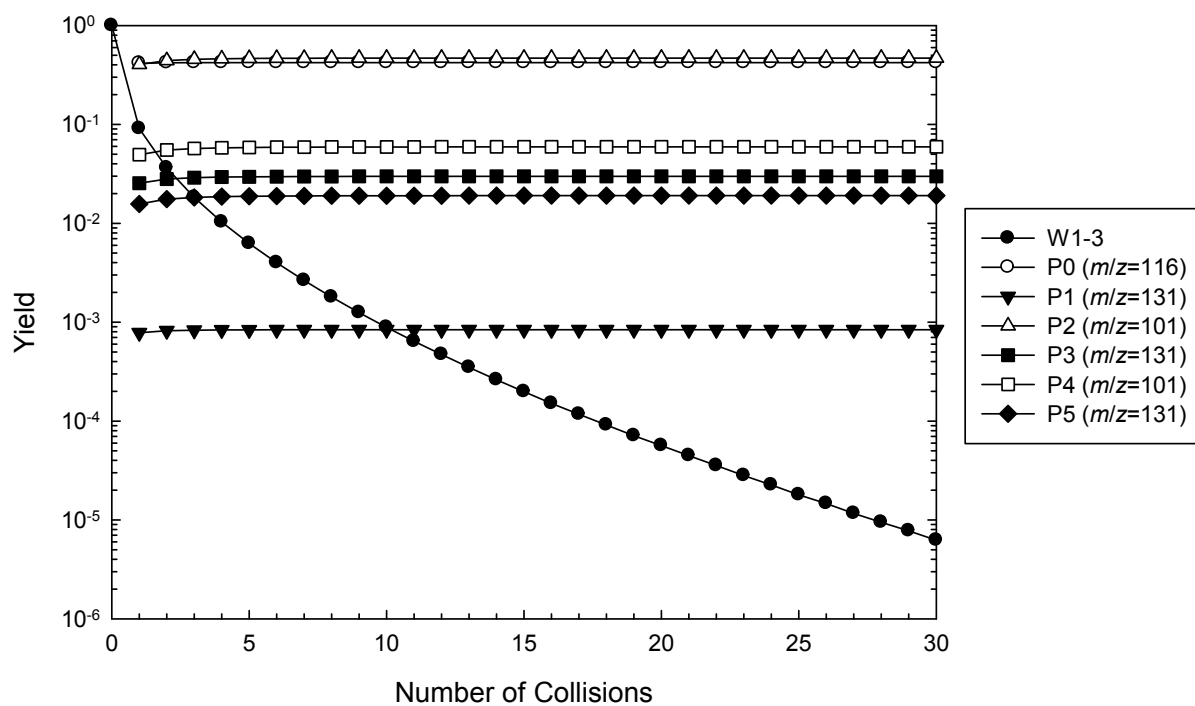


Figure S2. Master equation simulation for the $\text{CH}_2\text{C}(\text{OH})(\text{CH}_3)\text{CH}_2\text{COO}^- + \text{O}_2$ reaction system, using G3SX barrier heights at 307 K and 2.5 mTorr of helium. Results are presented as yields of wells and products as a function of number of collisions.

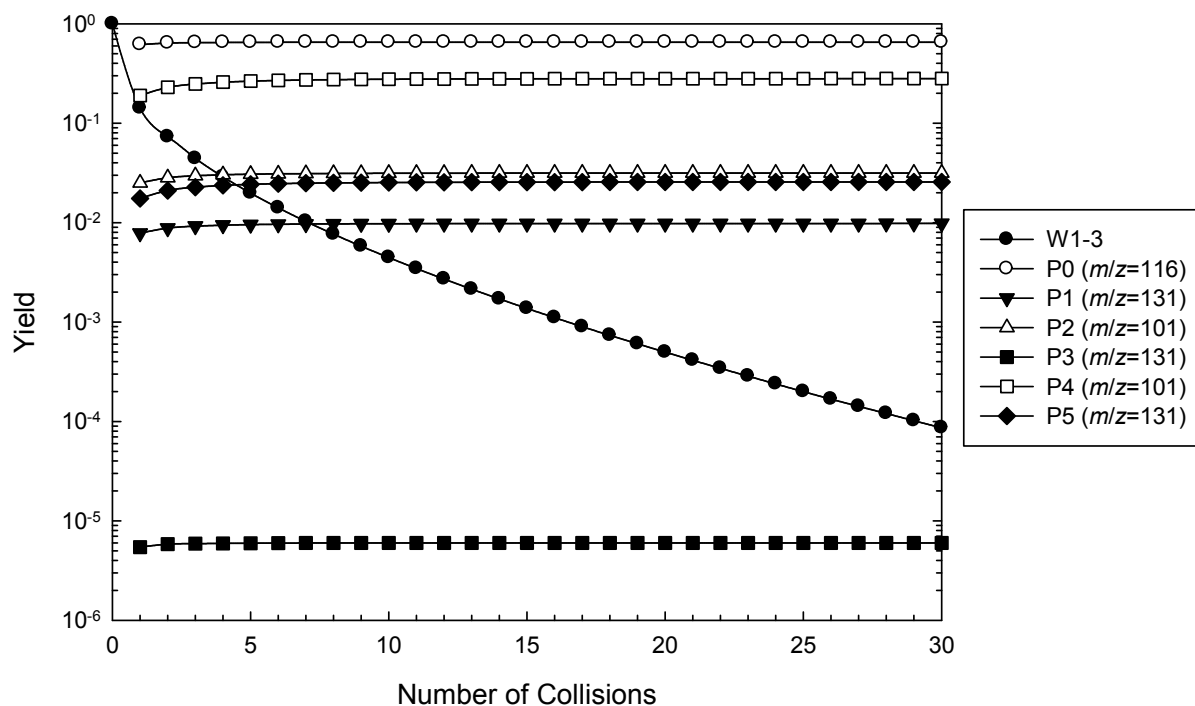


Figure S3. Master equation simulation for the $\cdot\text{CH}_2\text{C}(\text{OH})(\text{CH}_3)\text{CH}_2\text{COO}^- + \text{O}_2$ reaction system, using M06-2X/aug-cc-pVTZ barrier heights at 307 K and 2.5 mTorr of helium. Results are presented as yields of wells and products as a function of number of collisions.

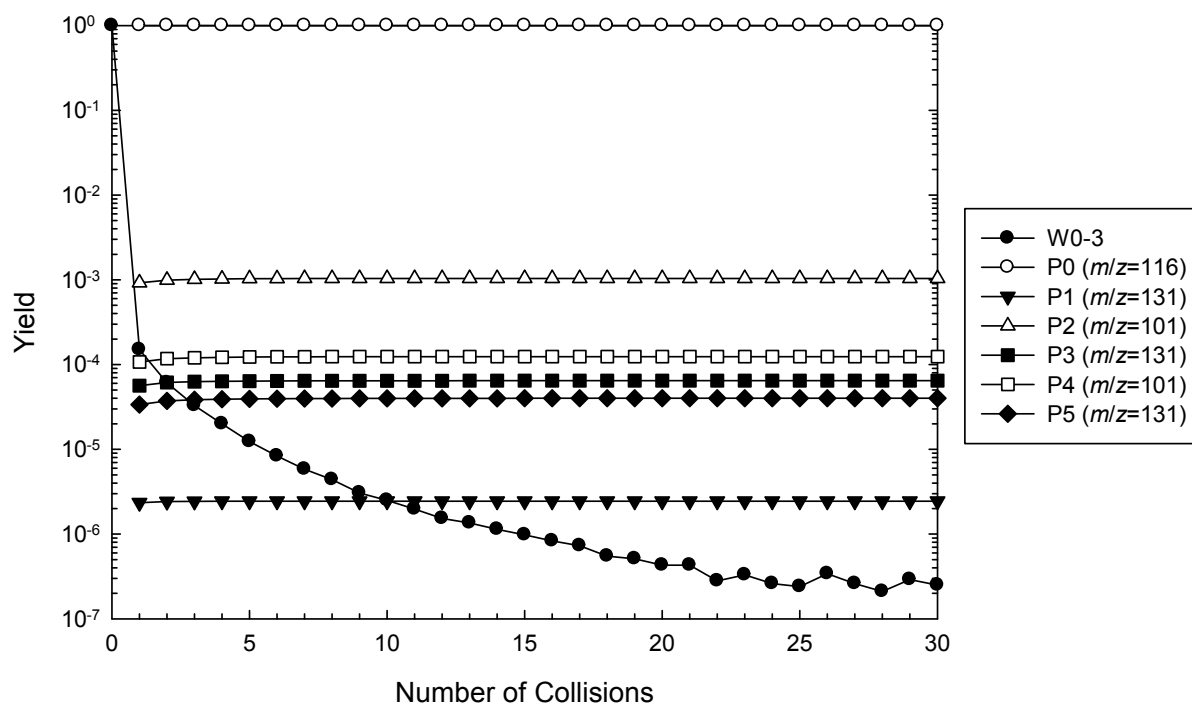


Figure S4. Master equation simulation for the $^{\bullet}\text{CH}_2\text{C}(\text{OH})(\text{CH}_3)\text{CH}_2\text{COO}^- + \text{O}_2$ reaction system, including the pre-reaction complex **W0** using G3SX barrier heights at 307 K and 2.5 mTorr of helium. Results are presented as yields of wells and products as a function of number of collisions.

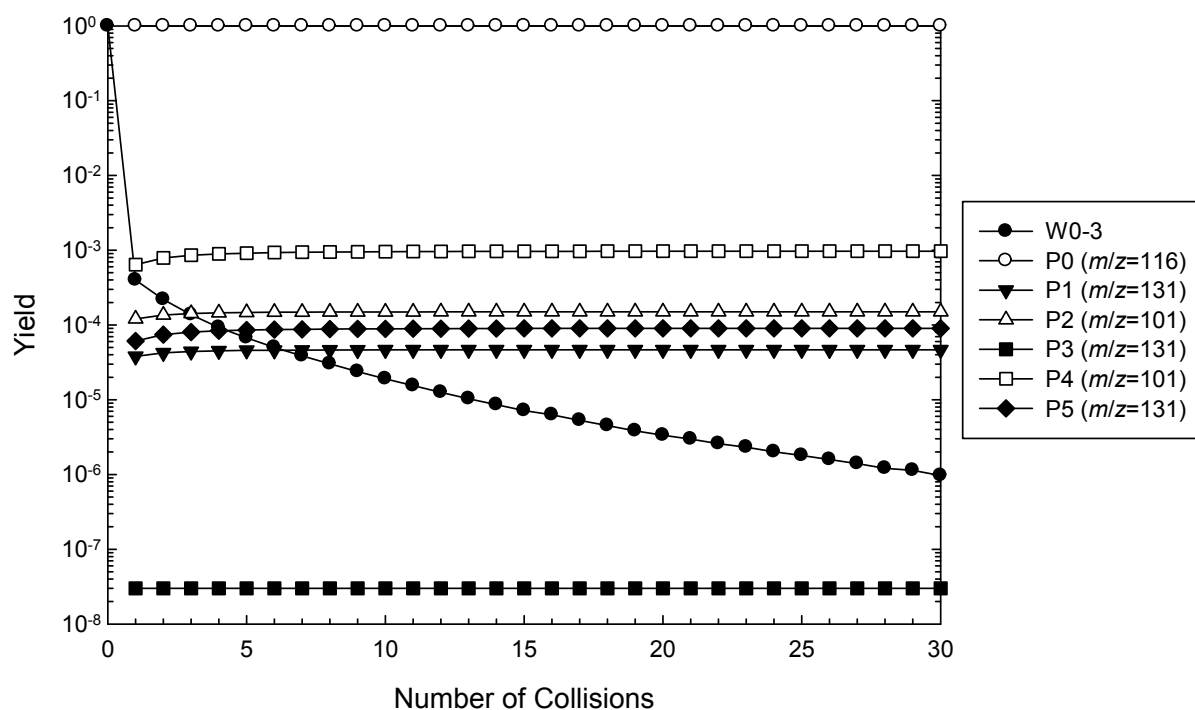
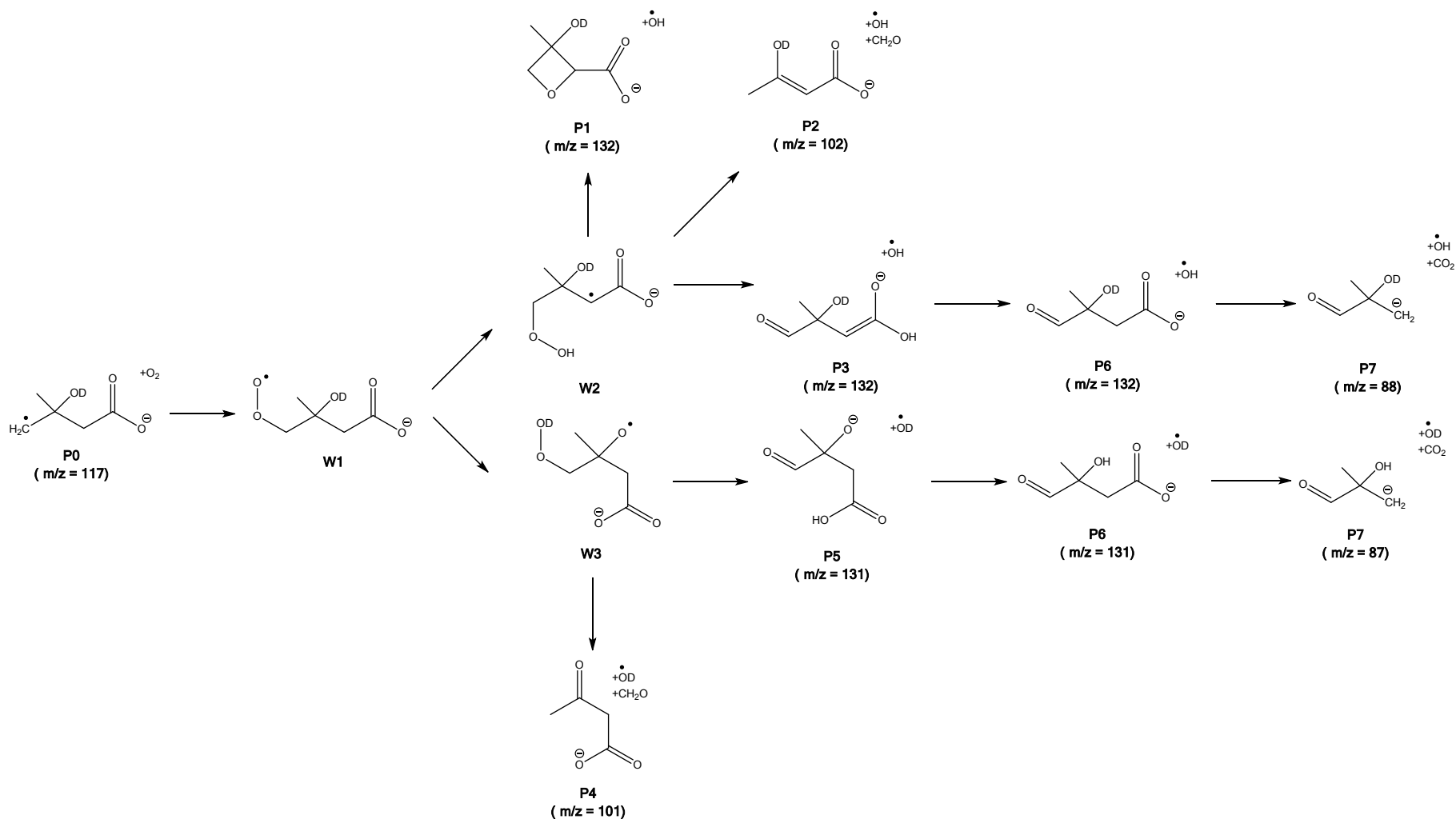
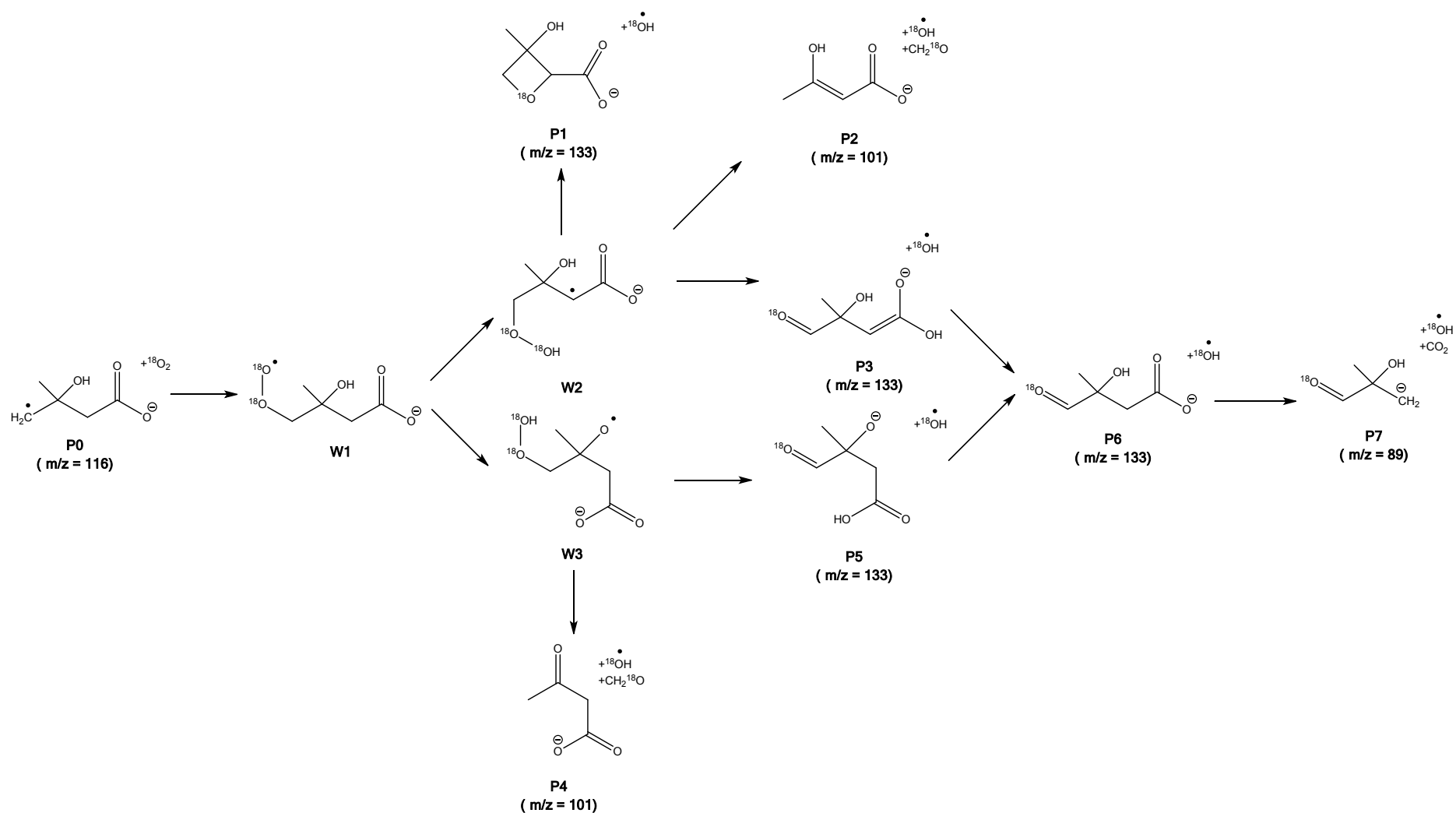


Figure S5. Master equation simulation for the $\cdot\text{CH}_2\text{C}(\text{OH})(\text{CH}_3)\text{CH}_2\text{COO}^- + \text{O}_2$ reaction system, including the pre-reaction complex **W0** using M06-2X/aug-cc-pVTZ barrier heights at 307 K and 2.5 mTorr of helium. Results are presented as yields of wells and products as a function of number of collisions.



Scheme S1. The reaction scheme for the $^{\bullet}\text{CH}_2\text{C}(\text{OH})(\text{CH}_3)\text{CH}_2\text{COO}^- + \text{O}_2$ reaction system using the deuterated isotopologue $^{\bullet}\text{CH}_2\text{C}(\text{OD})(\text{CH}_3)\text{CH}_2\text{COO}^-$, with m/z values for the wells and products provided.



Scheme S2. The reaction scheme for the $^\bullet\text{CH}_2\text{C}(\text{OH})(\text{CH}_3)\text{CH}_2\text{COO}^- + \text{O}_2$ reaction system using the $^{18}\text{O}_2$ isotopoe to replace O_2 , with m/z values for the wells and products provided.

Optimized Geometries – M06-2X, Å

W0	6-31+G(2df,p)		
C	-1.38041500	-0.28192000	-0.04257000
H	-2.19616200	0.23101000	0.45890300
H	-1.35951300	-0.25566200	-1.12751200
C	-0.11061500	-0.58938500	0.69198000
C	0.53907500	-1.86731200	0.12753100
H	0.64831700	-1.74336000	-0.95839200
H	-0.09690800	-2.73938200	0.30319200
C	1.95671100	-2.15897000	0.69749600
O	2.28328200	-3.34586600	0.80926400
O	2.65216900	-1.13534000	0.96935100
O	0.76318400	0.51057500	0.49286900
H	1.66326900	0.09592000	0.67194900
O	-2.89159900	-2.54771200	0.40289100
O	-3.62377100	-2.41928900	1.33880900
C	-0.39121900	-0.75616500	2.19071300
H	-0.81614100	0.17161100	2.58878300
H	-1.09122600	-1.57882600	2.37723100
H	0.54700300	-0.96466700	2.71257600

W1	6-31G(2df,p)		
C	-1.62483700	0.43157500	-0.75369700
H	-2.26363300	1.25886900	-0.43507600
H	-1.46708500	0.45719000	-1.83507100
C	-0.27239400	0.48572700	-0.04213100
C	0.65442500	-0.64023700	-0.52272600
H	0.66329200	-0.63407500	-1.62109000
H	0.30020000	-1.62236000	-0.19932200
C	2.13331900	-0.45438600	-0.05595600
O	2.80895200	-1.47162900	0.08052800
O	2.49317300	0.75217800	0.10637700
O	0.24798600	1.73328300	-0.41821500
H	1.23985800	1.57711800	-0.24519400
O	-2.33976300	-0.79409000	-0.49716200
O	-3.16026900	-0.68570200	0.49976800
C	-0.45738800	0.41825200	1.47720200
H	-1.09198900	1.24467900	1.81119800
H	-0.90870200	-0.52552100	1.79685200
H	0.52855100	0.52116700	1.93756100

W2	6-31G(2df,p)		
C	1.13473400	0.14935600	-1.04525400
H	0.68556800	-0.74675400	-1.49169000
H	1.18911200	0.94919700	-1.79423100
C	0.28393400	0.59340700	0.16889300
C	-1.12840800	0.80554900	-0.29348000
H	-1.36368700	1.68766600	-0.88068600
H	1.78281800	-1.22592500	0.65625400
C	-2.19894500	-0.22576600	-0.12304700
O	-3.29921300	-0.00614300	-0.63150300
O	-1.84640100	-1.26002900	0.54715600
O	0.35028200	-0.41759200	1.15247900
H	-0.56885000	-0.93810800	1.00256200
O	2.47300000	-0.12039600	-0.68261100
O	2.49477400	-1.37831000	-0.01295400
C	0.87888800	1.87464900	0.75924900
H	1.92705200	1.69861400	1.01459600
H	0.82088400	2.70367700	0.04575300
H	0.32727900	2.14380200	1.66249600

W3	6-31G(2df,p)		
C	-1.48040500	-0.85370900	-0.60631600
H	-1.48765900	-0.56128500	-1.66462400
H	-1.49483600	-1.94724900	-0.51842100
C	-0.22150900	-0.27713000	0.07771900
C	1.03247400	-0.75916700	-0.64150600
H	0.91827700	-0.59256800	-1.71996900
H	1.27192700	-1.81478300	-0.48081900
C	2.21277600	0.12314300	-0.17261000
O	3.36157200	-0.29454400	-0.29420600
O	1.85572800	1.24788800	0.30442400
O	-0.27761900	1.09382500	-0.06550400
H	-1.96584100	1.32176400	-0.02898500
O	-2.67207800	-0.42369500	0.01325500
O	-2.84824400	0.95447700	-0.28673800
C	-0.20748300	-0.68498000	1.55747300
H	-0.12474200	-1.77127200	1.68125600
H	0.64378400	-0.19997700	2.03857800
H	-1.13089800	-0.34718600	2.03457300

P0	6-31G(2df,p)		
C	-2.27161200	-0.73589000	-0.53155600
H	-2.65266400	-0.46069600	-1.50777300
H	-2.56118100	-1.69399600	-0.11237000
C	-1.05248700	-0.03977800	-0.02666300
C	0.21587600	-0.81886800	-0.45771100
H	0.18464400	-0.92693400	-1.54949400
H	0.23120100	-1.82391800	-0.02548200
C	1.55170100	-0.09212900	-0.09327100
O	2.53148900	-0.80956800	0.11301400
O	1.48747600	1.17176400	-0.07224100
O	-1.01399400	1.25036500	-0.58626800
H	-0.04754400	1.48597400	-0.45884700
C	-1.09308800	0.05858300	1.50936300
H	-1.96389300	0.64627300	1.81430800
H	-1.15209300	-0.93142000	1.97569000
H	-0.18423800	0.56112400	1.85006600

P1	6-31G(2df,p)		
C	-0.16724200	0.46167800	-0.59188400
C	1.71736900	1.01002300	-0.10631300
H	2.28911700	1.05179000	-1.04665000
C	-1.56337000	-0.00115100	-0.14102600
O	-1.64848900	-1.23435400	-0.39350500
O	-2.35638900	0.77828800	0.38447900
O	0.47075100	1.70739700	-0.20404000
H	2.33547200	1.36720300	0.72775400
C	0.97559300	-0.32403800	0.05032700
C	0.70920100	-0.65975500	1.50948400
H	0.34185800	0.22664000	2.03451200
H	-0.06148400	-1.43267200	1.55599300
H	1.62741500	-1.01857200	1.98676900
O	1.40636200	-1.44952100	-0.66800900
H	0.55651700	-1.88210500	-0.85202500
H	-0.09675700	0.34834300	-1.68546200

P2	6-31G(2df,p)		
C	-1.11062700	0.01436800	-0.00023500
C	0.02341900	-0.77583200	-0.00046100
H	-0.04831200	-1.85480500	-0.00072000
C	1.35917700	-0.20335000	-0.00004500
C	-2.47301900	-0.66810300	0.00028700
H	-2.40094100	-1.75826400	-0.00163500
H	-3.03777400	-0.34569100	0.88124000
H	-3.04019500	-0.34240500	-0.87783400
O	-1.13195500	1.28495300	-0.00018200
H	0.43479600	1.44169500	0.00008500
O	1.39731400	1.14309500	0.00019700
O	2.39698100	-0.84592700	0.00018300

P3	6-31G(2df,p)		
C	-1.30498300	0.69285600	-0.86045400
H	-1.43964700	0.30003700	-1.90127900
C	-0.89568500	-0.40077500	0.11503800
C	0.47550700	-0.77713300	-0.39241000
H	0.57263400	-1.60149400	-1.08972900
C	1.56527700	-0.02772400	0.02251900
O	2.81801800	-0.38482900	-0.48453300
O	1.57200900	0.92276400	0.82239600
O	-0.90395300	0.07582600	1.43385300
H	-0.08081600	0.60495900	1.48429100
O	-1.39156000	1.87127900	-0.62834700
C	-1.86800500	-1.56926200	0.02253200
H	-2.84803800	-1.28234700	0.41705900
H	-1.98345600	-1.90096900	-1.01496800
H	-1.47236600	-2.40106600	0.61150800
H	2.66291500	-1.10720200	-1.09718200

P4	6-31G(2df,p)		
C	-0.11362000	-0.63353000	0.67041500
H	-0.12743900	-0.26403800	1.70279300
H	-0.28556900	-1.70925400	0.66104200
C	-1.36603500	0.09274000	-0.04003600
O	-1.15687600	1.24817300	-0.44588000
O	-2.38700900	-0.59892700	-0.04714400
C	1.71536600	1.09393700	0.25926300
H	1.89884300	1.26187300	1.32625400
H	2.63629900	1.25290900	-0.30383200
H	0.90971500	1.76502000	-0.05375800
C	1.20637100	-0.31711600	0.04370700
O	1.83334300	-1.11458300	-0.62354900

P5	6-31G(2df,p)		
C	1.92925300	-0.74377900	-0.12139900
H	1.70545600	-1.83308600	-0.00470200
C	0.67186200	0.08353100	0.13140000
C	-0.43583800	-0.36249300	-0.90906800
H	-0.30867800	-1.42202300	-1.14771800
H	-0.42704800	0.23085600	-1.83083300
C	-1.76311600	-0.23886600	-0.22890500
O	-2.12625400	1.05485800	-0.03509800
O	-2.49313900	-1.13280800	0.10864300
O	0.35101900	-0.28666200	1.36899100
O	3.06953400	-0.35143600	-0.21853800
C	0.98877500	1.58128200	-0.04960600
H	1.33043400	1.82150100	-1.06493500
H	0.09714500	2.16866000	0.18187500
H	1.78315400	1.84428000	0.65272000
H	-2.93535000	1.00015100	0.48707200

P6	6-31G(2df,p)		
C	-0.69833500	0.25956500	0.01149900
C	0.38280500	-0.76644100	-0.39809800
H	0.21823800	-1.73240000	0.08560600
H	0.32508900	-0.91975200	-1.48451200
C	1.83615100	-0.27516400	-0.08461500
C	-1.99086300	-0.22690700	-0.60216100
H	-2.06765900	0.04913200	-1.67952600
O	2.67561500	-1.14600900	0.12810700
O	1.99338300	0.98137600	-0.11349100
O	-2.85374500	-0.86220700	-0.05394900
O	-0.42053700	1.50152600	-0.57376100
C	-0.81316300	0.35798200	1.53079500
H	-1.12400200	-0.59567100	1.96487600
H	0.15984000	0.64976900	1.93334400
H	-1.55073700	1.12110700	1.79469700
H	0.58770400	1.53802700	-0.47100100

P7	6-31G(2df,p)		
C	0.38694700	-0.01079400	0.00390600
C	0.34471700	1.47404900	0.33580100
H	0.07571400	2.05244200	-0.55332300
H	-0.39704100	1.66988700	1.11179200
H	1.33204500	1.79917100	0.68117000
C	0.64292100	-0.86968400	1.16627000
H	0.85779200	-1.91318700	0.94142500
H	1.18356900	-0.44564300	2.01106500
C	-0.98829900	-0.54777900	-0.23524400
H	-0.96115100	-1.63078200	-0.49482900
O	-2.05240700	0.05489000	-0.15358400
O	1.25197700	-0.19791900	-1.16564800
H	1.99479500	-0.66240400	-0.76784500

TS0	6-31+G(2df,p)		
C	-1.06179600	1.02927600	1.12176500
H	-1.79428700	1.63023900	1.65311800
H	-1.07310400	1.06837000	0.03706000
C	0.19760900	0.59390000	1.80826300
C	0.72180000	-0.71657500	1.19118800
H	0.79499200	-0.57859100	0.10390200
H	0.02954100	-1.54192600	1.37906300
C	2.13603300	-1.12723900	1.69230300
O	2.37823800	-2.33686300	1.76015300
O	2.91679900	-0.16489700	1.95871300
O	1.14899700	1.62588300	1.60595900
H	2.01991000	1.13245400	1.73869200
O	-2.66547300	-0.90840800	1.45275300
O	-3.40288700	-0.75006200	2.38619900
C	-0.05058600	0.41044500	3.31050400
H	-0.38161200	1.35959200	3.74540300
H	-0.81147900	-0.35527700	3.50076500
H	0.88317600	0.11022000	3.79444300

TS1	6-31G(2df,p)		
C	-1.87875500	0.51531600	-0.32529600
H	-2.49796800	1.31821400	0.09029400
H	-2.02034900	0.45661100	-1.41259600
C	-0.39710300	0.75010900	-0.00678200
C	0.37752600	-0.43475000	-0.55913500
H	0.31163500	-0.43167600	-1.65358100
H	-0.48499200	-1.40450000	-0.27110800
C	1.84661200	-0.53333500	-0.08874200
O	2.32160200	-1.57616200	0.33971000
O	2.37914500	0.60074200	-0.26248000
O	0.00037700	1.93843000	-0.66481200
H	0.97175900	1.82724200	-0.68640400
O	-2.31466400	-0.67237000	0.29836700
O	-1.66773600	-1.74883800	-0.31298100
C	-0.20734000	0.88824200	1.50437000
H	-0.78269400	1.74569000	1.86872500
H	-0.54353800	-0.01433200	2.02050700
H	0.85071200	1.05484300	1.71523600

TS2	6-31G(2df,p)		
C	-1.56937800	0.71520900	-0.25192300
H	-2.25078700	1.16710000	0.47669200
H	-1.83595500	1.04412500	-1.26604300
C	-0.09062200	0.92225100	0.02114700
C	0.39795300	-0.36893700	-0.58175700
H	0.20430600	-0.45069200	-1.64965600
H	-3.13343600	-1.91616100	0.16919800
C	1.75287200	-0.89665100	-0.12126100
O	1.94463300	-2.04215900	0.26297600
O	2.54789000	0.07737000	-0.26492900
O	0.47093800	2.04435100	-0.63239200
H	1.40742900	1.78643500	-0.68034900
O	-1.59494500	-0.69947600	-0.14165700
O	-3.25868300	-0.97723600	-0.00241700
C	0.17646900	0.98452700	1.52258700
H	1.25311300	0.93988200	1.69993700
H	-0.21895900	1.92454300	1.91955100
H	-0.30813500	0.14356800	2.02526700

TS3	6-31G(2df,p)		
C	1.10698800	-0.56220300	-0.51257200
H	0.59403100	-1.31938700	0.08831900
H	1.00544200	-0.69467000	-1.59613100
C	-0.05925200	0.92563000	0.07894400
C	-1.15712100	0.46947400	-0.69483100
H	-1.19956300	0.69274000	-1.75460100
H	3.17462200	-1.65229600	0.80702400
C	-2.16064500	-0.48404600	-0.11676100
O	-3.08221200	-0.87211900	-0.83248100
O	-1.93893500	-0.79946500	1.10821800
O	-0.10930100	0.76631300	1.40250400
H	-0.89797500	0.05146400	1.49481600
O	2.27004400	-0.13651100	-0.08247200
O	3.35757800	-1.38614100	-0.10152000
C	0.71198500	2.14870800	-0.35807300
H	1.68117200	2.16554600	0.14090800
H	0.86322300	2.15284300	-1.44023400
H	0.14506300	3.04054800	-0.07291500

TS4	6-31G(2df,p)		
C	0.69374400	-0.69996100	-0.64714500
H	-0.69027900	-1.36424300	-0.36529500
H	0.86995700	-0.60266700	-1.72935800
C	0.31178800	0.65841600	-0.01436300
C	-1.17783800	0.87263800	-0.05327500
C	-2.19887300	-0.19430500	-0.02044800
O	-1.76610000	-1.42649200	-0.15767400
O	-3.37742800	0.09214800	0.12533400
O	0.71966000	0.63590100	1.36314300
H	2.82181900	0.07377100	0.67936000
O	1.64789700	-1.35323600	0.01878800
O	3.05238900	-0.57025200	-0.00134700
H	-1.57155800	1.87957400	0.05006700
H	0.89536100	-0.30084900	1.53147000
C	1.01943700	1.84582400	-0.67081000
H	0.67661500	1.95692300	-1.70467900
H	0.80183100	2.77531400	-0.13093900
H	2.09535900	1.66195400	-0.68032400

TS5	6-31G(2df,p)		
C	1.47601700	1.08356000	0.06854600
H	1.47585100	1.51239200	-0.93827200
H	1.35306500	1.83813400	0.84846900
C	0.27534900	0.00554000	0.14637700
C	-0.95188900	0.80766300	-0.28089300
H	-0.85410600	1.08245400	-1.33630700
H	-1.05341300	1.72468800	0.30742900
C	-2.33760200	-0.00391200	-0.17427000
O	-3.29945700	0.77278100	-0.21808300
O	-2.24672700	-1.23033600	-0.10007500
O	0.61512500	-0.95972500	-0.73492900
H	1.81668700	-0.90007300	-0.83470300
O	2.66002500	0.41062100	0.31889000
O	2.89814400	-0.44238700	-0.74579400
C	0.17449900	-0.51433900	1.58090800
H	1.12576800	-0.96095600	1.88046300
H	-0.08214800	0.28888800	2.28026400
H	-0.61682900	-1.26423500	1.58857600

TS6	6-31G(2df,p)		
C	-0.82635100	-1.10472700	-0.19137900
H	-0.71357900	-1.15643800	-1.27165000
H	-0.09778200	-1.56475500	0.47078700
C	-0.25149200	0.92881400	0.05536000
C	1.14276100	0.85616700	-0.52760100
H	1.63376200	1.79810200	-0.23956400
H	1.06477300	0.87485900	-1.61737600
C	2.15872000	-0.28063900	-0.09933500
O	3.16854500	-0.31100100	-0.80847100
O	1.85453700	-0.98567600	0.88895100
O	-1.18401900	1.43872000	-0.62175300
H	-2.49072100	0.44842300	-0.63736700
O	-2.08959300	-1.12796700	0.26718700
O	-2.93856900	-0.44402900	-0.63882600
C	-0.35028800	0.95294900	1.57177400
H	0.37517300	0.26076900	1.99975300
H	-0.11212100	1.97468800	1.89290800
H	-1.37083500	0.72204700	1.88437100

TS7	6-31G(2df,p)		
C	-0.80711700	-0.76410000	-0.37966000
H	-0.98245000	-0.79115000	-1.46313900
H	0.34923600	-1.30951300	-0.02296700
C	-0.27069400	0.72975800	-0.00768300
C	1.13179600	0.80059100	-0.63297900
H	1.57978800	1.78004400	-0.44616300
H	1.01658100	0.69647400	-1.71883700
C	2.12514200	-0.27348400	-0.13924400
O	3.31296900	-0.00189800	-0.08317000
O	1.60723900	-1.41794500	0.16441600
O	-1.20022300	1.47440300	-0.59027300
H	-2.69319100	0.47846300	-0.37334800
O	-1.93545200	-1.07918700	0.31641400
O	-3.07210200	-0.42681000	-0.28228100
C	-0.22935600	0.85351300	1.51949900
H	0.45476300	0.12153500	1.95596300
H	0.10856300	1.86035700	1.78505300
H	-1.23136700	0.69761600	1.92298700

TS8	6-31G(2df,p)		
C	-1.13888400	0.86736900	-0.79261300
H	-1.28355500	0.61780500	-1.87167700
C	-0.88494500	-0.36199500	0.06707100
C	0.44707400	-0.91450200	-0.41680200
H	0.54830800	-1.95996900	-0.09563600
C	1.64511600	-0.13856300	0.08454700
O	2.49777500	-0.22273700	-0.91365000
O	1.80164500	0.48047800	1.13062500
O	-0.91277700	-0.02511400	1.43739400
H	-0.02045100	0.31680800	1.62416000
O	-1.15249200	2.00749900	-0.41516900
C	-2.02173200	-1.35049800	-0.18368000
H	-2.97410400	-0.94484900	0.17304000
H	-2.10118700	-1.59066000	-1.24763700
H	-1.80808800	-2.27117200	0.36568000
H	1.50177800	-0.69899800	-1.40956600

TS9	6-31G(2df,p)		
C	1.81636100	-0.81760200	0.01758500
H	1.48632800	-1.85896600	0.25071900
C	0.63538500	0.14031200	0.07854900
C	-0.44288900	-0.31966400	-1.00799100
H	-0.28650800	-1.35430800	-1.32728700
H	-0.46392800	0.33986400	-1.88178800
C	-1.73184100	-0.25626200	-0.25213800
O	-2.05945300	1.03490300	0.07235600
O	-2.41627400	-1.18101100	0.08138700
O	0.18552500	-0.03984600	1.32737800
O	2.99022500	-0.54302600	-0.07422200
C	1.09522800	1.57387700	-0.23968600
H	1.55917600	1.65925300	-1.23074700
H	0.22859600	2.23849100	-0.18605000
H	1.82690500	1.87569900	0.51354600
H	-2.18422200	1.00784700	1.02849700

OH	6-31G(2df,p)		
O	0.00000000	0.00000000	0.10803900
H	0.00000000	0.00000000	-0.86431000

O ₂	6-31G(2df,p)		
O	0.00000000	0.00000000	0.59497400
O	0.00000000	0.00000000	-0.59497400

CO ₂	6-31G(2df,p)		
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.15716000
O	0.00000000	0.00000000	-1.15716000

HCHO	6-31G(2df,p)		
C	-0.00000600	-0.52405000	0.00000000
H	0.93744400	-1.11340900	0.00000000
H	-0.93736000	-1.11358400	0.00000000
O	-0.00000600	0.67141100	0.00000000

Vibrational Frequencies – M06-2X, cm⁻¹

W0	W1	W2	W3
25.49	55.03	46.03	67.78
50.46	74.34	75.03	91.04
61.53	93.73	98.39	136.51
73.58	132.45	215.35	152.14
84.52	197.15	235.90	234.16
120.24	282.48	259.54	258.84
146.58	289.88	305.19	293.37
233.93	310.57	324.11	337.73
269.12	364.69	356.51	367.74
308.60	393.35	416.95	406.35
332.33	424.86	449.89	427.85
349.71	480.62	459.51	459.39
378.48	534.63	518.58	502.27
409.55	578.90	537.23	596.28
453.02	615.57	678.64	645.67
518.68	748.07	732.08	674.47
614.93	823.05	760.83	732.98
668.69	901.34	771.59	823.33
744.80	924.30	840.05	882.73
826.34	943.54	895.80	916.04
893.76	975.16	941.17	933.97
921.58	1004.86	967.05	958.90
936.57	1009.91	1000.42	999.94
948.26	1027.91	1005.81	1001.97
984.54	1128.13	1115.09	1119.84
990.82	1181.82	1131.39	1131.88
1112.85	1206.32	1154.86	1160.54
1180.86	1251.95	1171.60	1224.50
1211.92	1295.04	1220.40	1245.94
1271.04	1298.16	1296.57	1293.93
1291.16	1324.61	1326.96	1311.72
1379.95	1362.59	1364.34	1347.41
1396.36	1393.50	1380.45	1372.77
1438.16	1406.24	1391.01	1386.44
1445.33	1449.78	1453.56	1444.59
1468.03	1466.85	1483.69	1453.28
1490.97	1478.40	1494.61	1484.03
1530.38	1504.44	1586.32	1500.19
1715.98	1577.69	1633.60	1601.49
1731.73	1796.84	1790.19	1740.25
2990.18	2827.82	2189.52	3041.62
3038.48	3033.66	3043.88	3044.29
3043.00	3052.28	3049.18	3051.23
3107.16	3081.69	3109.96	3105.77
3122.46	3118.76	3132.43	3111.86
3135.14	3134.69	3155.68	3128.27
3150.21	3155.15	3207.69	3163.25
3257.80	3157.15	3336.34	3311.05

TS0	TS1	TS2	TS3	TS4
-72.17	-1737.69	-840.54	-1046.68	-446.98
17.06	70.10	58.54	57.28	71.39
45.73	118.20	96.06	69.61	85.97
59.43	157.09	108.30	101.64	142.22
72.04	185.63	173.98	117.11	183.12
113.09	248.50	183.67	175.38	266.75
150.30	282.36	221.90	193.77	278.80
229.32	300.06	240.47	231.63	309.61
261.46	340.97	294.65	261.42	334.57
310.88	387.41	306.26	272.70	358.96
352.12	425.73	316.49	280.18	382.39
360.80	461.84	345.79	321.53	419.60
381.31	486.09	400.67	341.68	469.35
413.62	547.87	477.41	402.02	514.84
453.61	607.41	503.75	448.99	542.92
521.89	662.13	551.49	522.28	553.55
615.29	740.06	645.30	583.86	588.93
701.13	778.40	663.02	674.69	669.08
745.84	824.83	772.56	765.89	703.27
826.91	915.77	814.80	811.62	770.61
892.48	960.99	842.82	855.94	811.92
923.48	971.12	937.04	918.18	916.56
935.28	986.47	984.03	957.60	930.65
961.26	992.71	997.99	1009.04	953.58
982.64	1021.51	1019.52	1024.33	1017.56
993.25	1117.20	1023.99	1076.39	1071.25
1112.82	1159.43	1135.41	1087.10	1159.88
1181.60	1188.23	1165.10	1161.69	1195.76
1213.40	1225.29	1187.31	1179.78	1215.71
1270.71	1280.55	1206.76	1234.65	1225.82
1291.43	1288.63	1276.17	1239.82	1261.01
1378.40	1309.84	1308.21	1303.92	1297.90
1396.49	1355.30	1353.14	1374.95	1347.15
1439.00	1370.24	1375.11	1393.71	1369.51
1445.14	1393.04	1385.45	1438.00	1376.97
1466.38	1456.18	1448.71	1475.05	1432.18
1490.18	1471.20	1495.67	1483.28	1483.87
1532.61	1497.91	1504.90	1528.50	1493.72
1656.83	1504.81	1521.92	1592.11	1604.43
1732.59	1587.38	1793.26	1788.37	1679.31
2933.98	1794.45	3032.80	2213.22	1872.30
3036.78	3046.92	3057.82	3044.26	3006.33
3044.62	3051.03	3100.75	3056.79	3031.92
3115.70	3081.74	3145.99	3135.75	3111.06
3119.71	3113.17	3160.03	3137.74	3154.84
3133.46	3135.82	3161.31	3165.46	3197.05
3143.80	3164.29	3694.08	3208.45	3771.51
3252.52	3550.37	3886.47	3861.49	3830.39

TS5	TS6	TS7	TSgor	TSgorPre
-1550.29	-335.45	-1266.56	62.62	62.62
45.48	37.10	71.15	132.23	132.23
72.71	86.41	132.76	208.09	208.09
108.01	138.05	159.49	237.95	237.95
165.31	170.67	192.55	274.21	274.21
234.24	230.99	215.57	305.89	305.89
256.80	241.75	278.90	351.35	351.35
302.09	254.33	306.11	371.86	371.86
338.65	269.96	327.84	403.53	403.53
352.82	317.53	392.02	454.81	454.81
441.62	355.83	422.86	497.95	497.95
459.66	402.83	443.13	549.37	549.37
530.95	452.75	483.30	624.94	624.94
588.14	534.31	545.33	745.16	745.16
612.51	555.05	607.19	819.00	819.00
677.85	585.50	639.05	899.33	899.33
706.56	671.84	652.65	906.83	906.83
762.24	733.58	668.77	913.12	913.12
799.11	758.68	769.52	967.59	967.59
819.94	820.47	845.40	988.42	988.42
909.87	882.22	916.59	999.39	999.39
928.07	898.10	930.02	1113.58	1113.58
972.06	915.23	934.21	1143.57	1143.57
998.30	989.41	998.47	1219.72	1219.72
1034.08	1023.85	1042.61	1272.69	1272.69
1064.49	1037.04	1066.73	1293.81	1293.81
1120.27	1148.58	1138.38	1373.39	1373.39
1135.56	1190.69	1183.73	1400.19	1400.19
1192.02	1227.82	1228.49	1426.04	1426.04
1205.91	1243.45	1259.00	1447.35	1447.35
1258.39	1249.91	1316.71	1477.50	1477.50
1296.33	1371.20	1335.92	1499.35	1499.35
1323.41	1398.88	1383.86	1573.19	1573.19
1351.98	1426.88	1404.72	1788.52	1788.52
1375.90	1464.94	1423.89	3040.19	3040.19
1432.60	1474.48	1456.72	3044.22	3044.22
1459.61	1504.60	1491.37	3065.83	3065.83
1478.10	1545.54	1496.50	3103.94	3103.94
1503.74	1636.58	1561.83	3125.63	3125.63
1789.80	1801.41	1673.80	3146.56	3146.56
1828.06	3022.55	1819.30	3149.60	3149.60
3043.95	3042.23	3054.27	3259.85	3259.85
3058.16	3119.49	3060.48	1791.53	1791.53
3075.21	3124.27	3064.46	11.33	11.33
3122.60	3129.79	3125.35	9.28	7.75
3129.35	3168.62	3138.91	295.61	246.97
3165.42	3192.42	3168.23		
3174.93	3281.48	3398.83		

Moments of Inertia – M06-2X, amu Å²

	W0	W1	W2	W3
<i>K</i> -Rotor	266.64	197.44	208.32	158.63
<i>J</i> -Rotor	767.17	678.52	642.33	671.77

	TS0	TS1	TS2	TS3	TS4
<i>K</i> -Rotor	254.36	259.67	267.71	245.85	205.50
<i>J</i> -Rotor	753.72	533.16	598.46	707.20	645.91

	TS5	TS6	TS7	TSgor	TSgorPre
<i>K</i> -Rotor	159.91	218.78	189.18	197.44	197.44
<i>J</i> -Rotor	703.20	649.34	637.22	489.95	552.11