

Conformations of favorable transition states in the thermal pyrolysis of alkyl acetates and xanthates

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Electronic Supporting Information

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1. Details of Calculations

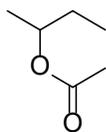
All calculations were performed with the Gaussian 09¹ and Multiwfn² programs. Density functional theory (DFT) calculations using the M06-2X theoretical method were used to locate all the stationary points involved.³ Structural optimizations were obtained at the M06-2X/def2-TZVP level (gas phase), while frequency calculations were under the same level and the substrates, intermediates, and products were characterized by no imaginary vibrational mode, but transition states were characterized by only one.⁴ Intrinsic reaction coordinate (IRC) calculations for typical transition states were performed, which assisted in confirming the transition states.⁵ Single-point energies were obtained at the level M06-2X/def2-TZVPP (gas phase). The contribution of vibration to entropy was calculated using a quasi-rigid-rotor-harmonic-oscillator (quasi-RRHO) approximation, which uses the Grimme method⁶ implemented in the Shermo program,⁷ switching to a free rotor description of vibrational modes below 100 cm⁻¹. The relative Gibbs free energies were corrected with quasi-RRHO and the scale factor of 0.971 was employed for ZPE.⁸ The change of concentration of substances with time was calculated using the concvar program.⁹

All wavefunction analyses including Mayer bond order,¹⁰ orbital isosurface¹¹ were calculated using the Multiwfn program. All the presented structures were visualized by CYLview20 program,¹² and the orbital isosurface and electrostatic potential were created by the Multiwfn and VMD 1.9.3 program.¹³

References

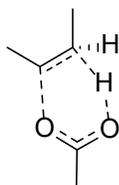
- 1 Gaussian 09, Revision B.01: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian, Inc., Wallingford, CT, 2009.
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J. L. Bao, J. Zheng, I. M. Alecu, B. J. Lynch, Y. Zhao and D. G. Truhlar, Database of Frequency Scale Factors for Electronic Model Chemistries (Version 3 Beta 2), <https://comp.chem.umn.edu/freqscale/version3b2.htm>.
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2. Coordinates of All Stationary Points



1

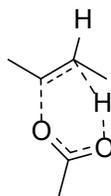
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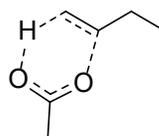
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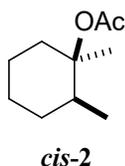
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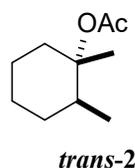
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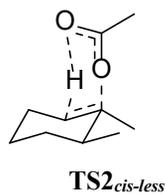
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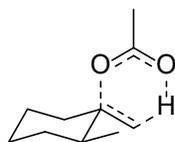


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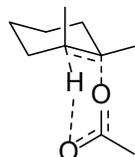
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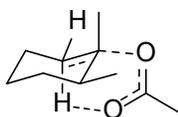
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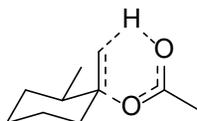
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C	-3.34250300	-0.86239000	-0.44309300
H	-3.05622800	-1.68863700	-1.09667100
H	-3.75016200	-1.27244700	0.47767800
H	-4.08260400	-0.25882000	-0.96385100
O	-1.78926900	0.86368600	-0.97911400



TS2_{trans-less}

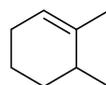
C	2.48553500	0.85707300	-0.27902600
C	3.03636300	-0.54182000	-0.54213000
C	2.30534200	-1.58917200	0.29409600
C	0.78667800	-1.51600000	0.04698100
C	0.35978800	-0.12255200	0.38009700
C	0.96050900	0.92503900	-0.50950800
H	2.65795600	-2.59311400	0.05387400
H	2.91478500	-0.78175800	-1.60294300
H	4.10677500	-0.57068200	-0.33022300
H	2.70066400	1.15402400	0.75285400
H	2.96465300	1.59239900	-0.92894500
H	0.57452900	-1.72721900	-1.00100800
H	0.25349600	-2.23894200	0.66445600
H	0.76304900	0.61493600	-1.53830200
H	2.50833300	-1.42049200	1.35567600
C	-0.07491400	0.18697300	1.68373500
H	0.20348200	1.16060700	2.07487400
H	-1.31763700	0.38702900	1.41751400
H	-0.04572600	-0.62423600	2.40443700
C	0.40770900	2.32451400	-0.29518800
H	0.76688200	2.98966900	-1.08094800
H	-0.68257400	2.31479800	-0.31882900
H	0.72926600	2.74203800	0.66047300
O	-1.37656200	-0.26948500	-0.78378500
C	-2.46511300	-0.12694500	-0.17867700
O	-2.56858600	0.47145500	0.93137800
C	-3.71538800	-0.72480700	-0.77586400
H	-3.89850700	-1.68666000	-0.29364200
H	-4.56729500	-0.07908800	-0.57323000
H	-3.59000300	-0.88288900	-1.84393000



TS2_{trans-term}

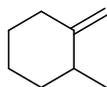
C	2.39005200	0.01978500	-0.76804000
C	2.12503200	-1.47855200	-0.72733200
C	1.53777100	-1.88415800	0.61870300
C	0.43690300	-0.93454500	1.10589100
C	0.45294900	0.42818100	0.72121500
C	1.06585000	0.78399200	-0.60919700
H	1.14387400	-2.90008000	0.57139200
H	1.42449700	-1.73370000	-1.52676800

H	3.04258400	-2.04068100	-0.90968600
H	3.09138100	0.30727800	0.02401000
H	2.84577400	0.31106900	-1.71616200
H	-0.54969700	-1.22883300	0.42744200
H	0.16499800	-1.08676300	2.14851400
H	0.37924800	0.36932200	-1.35183800
H	2.33531700	-1.89038800	1.36815700
C	0.20709100	1.48271900	1.73610800
H	-0.23152200	2.38010200	1.31249400
H	-0.41762700	1.10662500	2.54303100
H	1.19021300	1.73534300	2.15570300
C	1.20167600	2.27693900	-0.86385600
H	1.63658100	2.44071000	-1.85001900
H	0.22820700	2.76514500	-0.83829400
H	1.85428600	2.75464200	-0.12972500
O	-1.59445500	0.79778200	-0.02949700
C	-2.24053800	-0.24293400	-0.29598000
O	-1.71096800	-1.38619800	-0.40310200
C	-3.73998300	-0.14636500	-0.46616000
H	-4.06240100	-0.80437600	-1.27098700
H	-4.21379100	-0.48898500	0.45527500
H	-4.03934500	0.88051700	-0.65985900



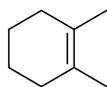
3

C	0.77176500	-1.37408200	-0.07754600
C	1.95102500	-0.52543900	0.37567700
C	1.88979900	0.84263000	-0.29434500
C	0.50673500	1.42564300	-0.22296900
C	-0.59325400	0.73708600	0.07586700
C	-0.56217900	-0.75616200	0.34041000
H	2.59782200	1.53059700	0.17428000
H	1.90526000	-0.39791100	1.46152300
H	2.89676400	-1.02037700	0.14880700
H	0.79010400	-1.45852400	-1.17034100
H	0.84181500	-2.38911500	0.32020600
H	0.41469700	2.49117000	-0.41380200
H	-0.68052800	-0.89273500	1.42435800
H	2.20122400	0.75889400	-1.34196100
C	-1.92925400	1.41476200	0.19280900
H	-2.40246300	1.17300700	1.14905600
H	-1.82677500	2.49686000	0.12468300
H	-2.61520800	1.08639800	-0.59118200
C	-1.71852900	-1.48751300	-0.34333600
H	-1.62654300	-2.56367600	-0.18719000
H	-2.68904000	-1.17566700	0.04200400
H	-1.70377600	-1.30046900	-1.41984400



4

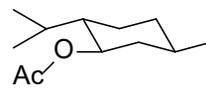
C	0.22194400	-1.44404000	-0.33632500
C	1.66692200	-1.09344200	0.00427800
C	1.95623200	0.37772500	-0.27729000
C	0.96374700	1.27709800	0.46642400
C	-0.45532500	0.90026300	0.13064700
C	-0.78478100	-0.54951500	0.40555300
H	2.97884100	0.62970300	0.01019900
H	1.84581100	-1.29834600	1.06535100
H	2.35158200	-1.72995200	-0.55984900
H	0.05986000	-1.32277100	-1.41323700
H	0.01745000	-2.49075300	-0.09797800
H	1.12005700	1.15080900	1.54428000
H	1.14048300	2.32760600	0.23236500
H	-0.62056000	-0.70954000	1.48016500
H	1.86666400	0.56522400	-1.35166800
C	-1.30516600	1.77019400	-0.40288500
H	-2.32102600	1.50416800	-0.66300700
H	-1.00332900	2.79294000	-0.59449900
C	-2.21421400	-0.94730000	0.07425700
H	-2.38230300	-1.99477000	0.32820300
H	-2.93745800	-0.34460700	0.62467900
H	-2.41222400	-0.82560100	-0.99294900



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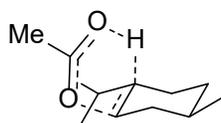
C	-1.89041700	0.66649900	-0.36741600
C	-1.89042600	-0.66649300	0.36740300
C	-0.66166500	-1.47099800	-0.03290900
C	0.61850500	-0.66711200	-0.02952000
C	0.61850800	0.66711000	0.02952800
C	-0.66166200	1.47099900	0.03292300
H	-0.53420900	-2.32833100	0.63581500
H	-1.86798500	-0.47972500	1.44550300
H	-2.79915800	-1.23316100	0.15740600
H	-1.86795200	0.47973200	-1.44551500
H	-2.79915300	1.23316800	-0.15743700
H	-0.80498700	1.89789600	1.03342600
H	-0.53420100	2.32834700	-0.63578100
H	-0.80498000	-1.89791900	-1.03340400
C	1.85288100	-1.52286100	-0.09811400
H	1.73002200	-2.28168400	-0.87571600
H	2.75913600	-0.96609000	-0.31987300
H	2.00131500	-2.06202100	0.84207800

C	1.85288600	1.52285600	0.09810800
H	2.75914500	0.96608300	0.31984800
H	2.00130500	2.06202400	-0.84208200
H	1.73004000	2.28167300	0.87571800



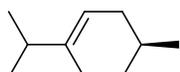
6

C	0.10872600	-0.34435600	0.04783000
C	-0.89963500	-1.42498300	-0.30459400
C	-2.26555000	-1.12510700	0.31016200
C	-2.72791100	0.26543400	-0.11983800
C	-1.69706700	1.34296900	0.20999000
C	-0.33310800	1.03712800	-0.41804400
H	-0.99350000	-1.47552000	-1.39550000
H	-0.52712100	-2.39084800	0.04361800
H	0.26269900	-0.34313700	1.12927900
H	-2.90603500	0.25471400	-1.20185800
H	-3.68389500	0.50212800	0.35384600
H	-2.05575700	2.31166200	-0.14029900
H	-1.59186500	1.41826500	1.29755800
H	-0.47579600	0.97922700	-1.50546900
H	-2.14848300	-1.11961900	1.40085400
C	-3.28275200	-2.19535200	-0.06126300
H	-2.95461200	-3.18332500	0.26542200
H	-4.25321300	-1.99183200	0.39440700
H	-3.42138500	-2.22857800	-1.14487200
C	0.73868100	2.11502700	-0.16515600
H	1.60131100	1.83193200	-0.77379900
C	0.27236400	3.48968300	-0.63919500
H	-0.48652600	3.90404200	0.02751100
H	1.10790700	4.19083000	-0.65751400
H	-0.15110500	3.44314200	-1.64499400
C	1.20581400	2.18492400	1.28790900
H	1.67899600	1.25768400	1.61468700
H	1.93684400	2.98637400	1.40709100
H	0.37528800	2.39882900	1.96441500
O	1.37110800	-0.63461700	-0.58054900
C	2.20226300	-1.46715900	0.06287200
C	3.46980400	-1.67189300	-0.71766200
H	3.23142400	-2.08293300	-1.69811900
H	3.96086400	-0.71161800	-0.87334300
H	4.12409300	-2.34629500	-0.17470800
O	1.95640400	-1.97076000	1.12476400



TS3

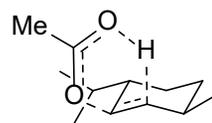
C	1.13974600	-0.46591700	-0.34992500
C	0.19571800	-0.50240300	0.81250500
C	-0.42492800	0.64873000	1.32716300
C	-0.35494600	1.99823600	0.60335000
C	0.72913900	2.01200200	-0.48446000
C	0.76044200	0.69934700	-1.26309800
H	-1.61708500	0.15418800	1.23023200
H	-0.09174700	2.75141100	1.34976000
H	0.54991200	2.84991600	-1.16171000
H	1.70873500	2.18285800	-0.02959700
H	-0.22658600	0.48954300	-1.68449800
H	1.44838600	0.76138700	-2.10567500
H	-0.44513600	0.68505300	2.41567100
O	-1.19542300	-1.57291900	-0.20223500
C	-2.37710200	-1.16899900	-0.07398900
O	-2.76025500	-0.46305600	0.90236100
C	-3.37483200	-1.48832400	-1.15817200
H	-3.06961600	-2.37273500	-1.71135000
H	-4.36385700	-1.61844000	-0.72434700
H	-3.41415300	-0.63852000	-1.84324900
H	0.29402400	-1.34313900	1.48619500
H	1.05909300	-1.40546300	-0.89987500
C	2.58437600	-0.39425800	0.22255000
H	2.61649500	0.37625400	0.99960900
C	2.98834200	-1.72639000	0.85417400
H	3.99685900	-1.66298200	1.26487900
H	2.32450800	-2.03000700	1.66305300
H	2.98304300	-2.51802400	0.10109400
C	3.59357300	-0.02029200	-0.86017700
H	4.60852400	-0.09160800	-0.46673900
H	3.51437600	-0.70407500	-1.70955800
H	3.45030700	0.99519600	-1.22819200
C	-1.71114700	2.39805800	0.01489400
H	-2.49917900	2.35575500	0.76709200
H	-1.66936200	3.41071500	-0.39003000
H	-2.00239800	1.72177900	-0.79265400



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C	0.17877400	1.13394500	-0.68336000
C	1.41503800	1.19817200	-0.20335500
C	2.13264000	0.03386000	0.42720800
C	1.39329000	-1.26759800	0.12437900

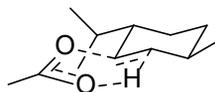
C	-0.10792800	-1.11960000	0.34911700
C	-0.70147600	-0.08657300	-0.61046700
H	1.96898000	2.12984900	-0.27906200
H	-0.25396100	2.01308800	-1.15442200
H	1.57641000	-1.53680500	-0.92209000
H	1.79927900	-2.07565200	0.73727300
H	-0.60704400	-2.08168800	0.22129400
H	-0.27959700	-0.80152200	1.38214000
H	-0.72303900	-0.53746400	-1.61254900
H	2.13636900	0.18404800	1.51465600
C	3.58482200	-0.02577100	-0.04034500
H	4.12231200	0.88757000	0.21985900
H	4.10625600	-0.86881800	0.41638300
H	3.62907000	-0.14558100	-1.12506100
C	-2.15808300	0.30648100	-0.29019300
H	-2.46054800	1.00714400	-1.07685900
C	-3.09269400	-0.89766400	-0.35447600
H	-2.88982400	-1.59375200	0.46211200
H	-4.13409400	-0.58409400	-0.26606000
H	-2.98076700	-1.43977300	-1.29582200
C	-2.30464000	1.02729000	1.04808800
H	-1.61494600	1.86861400	1.13005900
H	-3.32077800	1.40761100	1.16456900
H	-2.11254200	0.35196900	1.88400300



TS4

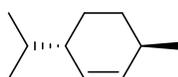
C	0.62692500	2.37620700	-0.00239300
C	-0.70674100	2.33367500	-0.75100700
C	-1.11953100	0.90537600	-1.10894500
C	-0.91693400	-0.10357500	0.02960500
C	-0.15957100	0.27477800	1.15660900
C	0.45974400	1.61955000	1.31308800
H	-2.17289500	0.90765700	-1.39460100
H	-1.47687200	2.78044000	-0.11375300
H	-0.65143300	2.93999800	-1.65766100
H	0.85296000	3.41658500	0.24510100
H	-0.03495600	-0.88356800	-0.37147600
H	-0.24500800	2.16841300	1.95469800
H	1.39253700	1.53561400	1.86956000
H	-0.57474700	0.57154700	-1.99642100
C	-2.05236800	-1.10630800	0.28967300
H	-1.66742600	-1.82701200	1.01898900
O	1.64026200	-0.72833000	1.14135600
C	1.89737900	-1.40369900	0.11273200
C	3.33503200	-1.77462800	-0.15541500
H	3.77458300	-0.98476000	-0.76859700

H	3.89151900	-1.84095000	0.77632100
H	3.38392200	-2.70824300	-0.71106700
O	1.02428600	-1.74703500	-0.73014100
C	-2.41902800	-1.88130100	-0.97337000
H	-3.16735200	-2.64280800	-0.74895500
H	-2.84235900	-1.22020100	-1.73252000
H	-1.54285300	-2.37254800	-1.39815200
C	-3.27760600	-0.42097200	0.89208900
H	-3.67625400	0.33348200	0.20949200
H	-4.07361800	-1.14224900	1.08617600
H	-3.03091300	0.07448000	1.83359300
H	-0.31936400	-0.27538900	2.07629400
C	1.77552100	1.83000200	-0.84730800
H	1.92059300	2.44832200	-1.73506300
H	2.70711100	1.81884300	-0.27957800
H	1.57952300	0.81062000	-1.18426100



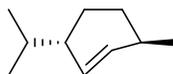
TS5

C	0.82814900	2.31496900	0.38323300
C	2.16758800	1.71264500	-0.12450200
C	2.28541900	0.18618000	0.03698700
C	1.04559000	-0.65585700	-0.49570600
C	0.02287100	0.16375500	0.16628900
C	-0.24856200	1.44990800	-0.29660000
H	3.16709800	-0.16897400	-0.49829000
H	2.25123900	1.96280000	-1.18757100
H	3.01842600	2.18453800	0.37645600
H	-0.01774200	0.02589800	1.24621200
H	-0.12953300	1.52633000	-1.38283500
H	-1.79279800	1.34778000	0.04069600
H	2.43329400	-0.05926000	1.09179500
O	-1.75642200	-0.99184600	-0.00103100
C	-2.78975200	-0.31648500	-0.03451800
O	-2.82338600	0.96689100	0.11834400
C	-4.12592500	-0.96360500	-0.27290000
H	-4.83272100	-0.62166400	0.48185100
H	-4.50020200	-0.64123700	-1.24506400
H	-4.03084000	-2.04505600	-0.25084600
H	0.77769000	2.18618400	1.46996900
C	0.71690100	3.79353600	0.04768400
H	-0.21173400	4.20864900	0.43843900
H	1.55367500	4.35894700	0.46375200
H	0.71959000	3.93492700	-1.03553400
H	0.99776600	-0.50883900	-1.57808500
C	1.11559900	-2.15412500	-0.17996200
H	0.27314700	-2.59898900	-0.71617100
C	2.40388900	-2.77304500	-0.71668200
H	3.26814800	-2.45993500	-0.12684600
H	2.35320400	-3.86155200	-0.67104200
H	2.58263500	-2.48736900	-1.75574400
C	0.92923200	-2.48199900	1.29912200
H	-0.05765900	-2.18214500	1.65074700
H	1.02339800	-3.55797600	1.45377100
H	1.68639100	-1.99867300	1.92116700



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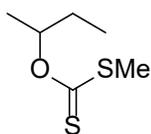
C	-0.09755600	-1.33515600	0.09408100
C	-1.59883700	-1.27929900	0.05768600
C	-2.14466000	0.12211500	0.32333700
C	-1.32569100	1.13656800	-0.46871200
C	0.13308700	1.12756000	-0.02533300
C	0.69915700	-0.26950400	0.06352500
H	-1.95361500	-1.62454000	-0.92233000
H	-2.01176800	-1.98317500	0.78629900
H	0.35441800	-2.32207300	0.14671500
H	-1.38682000	0.87984700	-1.53228600
H	-1.74883700	2.13774300	-0.35618500
H	0.73890800	1.72940000	-0.70826400
H	0.22310100	1.61054600	0.95445000
H	-2.00297800	0.34017800	1.38864400
C	-3.62875400	0.20969000	-0.00177100
H	-4.19960100	-0.54275500	0.54584500
H	-4.03273300	1.19152700	0.25059800
H	-3.79429900	0.04303700	-1.06934300
C	2.20435200	-0.41099000	0.10780100
H	2.42278800	-1.45482900	0.34956800
C	2.83790000	-0.10552100	-1.25243000
H	2.66871700	0.93324500	-1.54301000
H	3.91735700	-0.26353500	-1.21454600
H	2.42272600	-0.74782700	-2.02958900
C	2.82489800	0.46921100	1.19395600
H	2.37573300	0.27056000	2.16825800
H	3.89813500	0.28651700	1.26698800
H	2.68538600	1.52809400	0.96534900



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C	-2.27001800	-0.24803500	0.30938400
C	-1.44419900	1.10775700	0.37769700
C	0.09405600	0.97569800	0.45962400
C	0.75242400	-0.04458000	-0.57093800

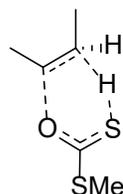
C	-0.19559900	-1.17856600	-0.31965400
C	-1.43847800	-0.90373000	-0.74820900
H	0.53108200	1.96585200	0.30909800
H	-1.70410700	1.67801200	-0.52000900
H	-1.79863100	1.69209000	1.23186600
H	-0.11568200	-1.58758600	0.68802200
H	-1.53530200	-0.42330700	-1.72379600
H	0.37163500	0.65763500	1.46826300
H	-2.15347700	-0.76277400	1.26671900
C	-3.73450600	0.01065400	0.00583800
H	-4.30011400	-0.92093400	-0.00893800
H	-4.18245700	0.67095400	0.75086200
H	-3.84144200	0.48621200	-0.97177000
H	0.59011100	0.36687200	-1.57224600
C	2.25509400	-0.26815300	-0.36764700
H	2.58283500	-0.86778100	-1.22280000
C	3.02709300	1.04951800	-0.39849800
H	2.83214900	1.63936200	0.49971500
H	4.10154100	0.86641600	-0.44397800
H	2.75031800	1.65376400	-1.26524300
C	2.58984100	-1.05741600	0.89515400
H	2.13512800	-2.04807300	0.88151100
H	3.66978600	-1.18795100	0.98148900
H	2.25238100	-0.53765100	1.79472700



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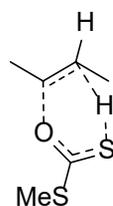
C	2.10063000	1.64722700	-0.80718200
H	1.72417200	2.17001400	0.06848600
H	3.17786100	1.80701000	-0.87425300
H	1.63685700	2.06505100	-1.70050800
C	1.84053700	0.15577300	-0.72228900
H	2.29116500	-0.33001500	-1.58959600
C	2.40085400	-0.50732300	0.52903400
H	3.48881400	-0.45774000	0.42796300
H	2.13593700	0.07040500	1.41299800
C	1.95757900	-1.95531700	0.68519400
H	2.17133700	-2.53364700	-0.21576600
H	2.47206300	-2.42761500	1.52143300
H	0.88530100	-2.01724600	0.87549700
O	0.44055000	-0.16113500	-0.95543800
C	-0.54803900	0.13448700	-0.13130300
S	-0.49506200	0.94917100	1.28479200
S	-1.99656700	-0.54272400	-0.85719300
C	-3.26318200	-0.07339600	0.32162100
H	-4.19561600	-0.46571400	-0.08126700

H	-3.05907700	-0.51186100	1.29508400
H	-3.31742100	1.00858100	0.41139100



TS6_{cis}

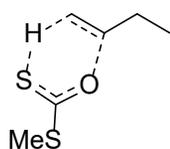
C	-2.09069500	1.74026000	-0.83555900
H	-2.14099000	0.97445700	-1.60945700
H	-3.10893200	2.10995400	-0.66755300
H	-1.46113500	2.55752300	-1.17437500
C	-1.59273900	1.15851500	0.43105800
H	-1.03353100	1.80782200	1.09129500
C	-2.07429700	-0.06104100	0.94304600
H	-1.21215800	-0.80941400	0.49860200
H	-1.95726700	-0.16714600	2.01859500
C	-3.32906800	-0.68786900	0.35621700
H	-3.22866400	-0.82842900	-0.71972900
H	-3.48876400	-1.67003800	0.79821200
H	-4.21317600	-0.07766500	0.54685800
O	0.33511700	0.83561600	-0.37529800
C	0.85182800	-0.28353300	-0.25653000
S	0.02306000	-1.76246500	-0.46906500
S	2.55183600	-0.41177400	0.22113000
C	3.00635000	1.33167600	0.25870700
H	2.44940700	1.85809000	1.02939200
H	4.07041500	1.36819000	0.48386800
H	2.81724100	1.79149600	-0.70798300



TS6_{trans}

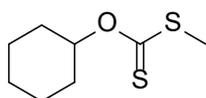
C	-2.42849900	1.48562900	-1.11760200
H	-2.56670800	0.68547100	-1.84479100
H	-3.40932000	1.91625900	-0.88877100
H	-1.79801900	2.26266200	-1.54161900
C	-1.85088000	0.95157800	0.13649500
H	-1.38127400	1.65758700	0.81108500
C	-2.14399900	-0.33937300	0.59790900
H	-3.05369800	-0.76215600	0.16910200
H	-1.35302500	-0.97188600	-0.10075300
C	-1.82942600	-0.70607000	2.03330500

H	-2.54771900	-0.27421700	2.73120900	C	-2.92314700	1.17999800	0.66126700
H	-1.83337400	-1.78737700	2.16243300	H	-1.53335200	-1.88427100	-1.37736700
H	-0.83229300	-0.34904900	2.29786700	H	-0.89562700	0.48459300	-1.10627300
O	0.14387900	0.88374100	-0.58033500	H	-1.51899400	0.02898700	1.83576300
C	0.73832800	-0.19821900	-0.48407000	H	-0.82750800	1.49764500	1.13807400
S	0.08577300	-1.70102700	-0.96255200	H	-3.32938200	-0.20466900	-1.72531500
S	2.34466100	-0.25038500	0.26375100	H	-4.00206900	-1.65948000	-1.01185500
C	2.62354600	1.50867500	0.53933600	H	-4.86723000	0.40668000	0.10978000
H	1.90268000	1.90656400	1.24902000	H	-3.97334600	-0.60896900	1.23037500
H	3.62892500	1.60221600	0.94518600	H	-2.89025300	1.86689100	-0.19081700
H	2.55143000	2.05326300	-0.39869200	H	-3.28858800	1.75430300	1.51380700



TS6_{term}

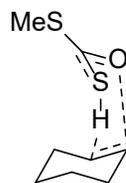
C	1.83168400	0.55267400	-1.47008700
H	2.74675000	1.07653800	-1.20955500
H	1.48924200	0.70366000	-2.48736000
H	1.03392400	1.21295700	-0.78603600
C	1.67520700	-0.73390300	-0.93655500
H	1.09406300	-1.45802100	-1.49360200
C	2.50351700	-1.27189300	0.17260300
H	1.94235900	-2.06559200	0.66468900
H	3.36658600	-1.75289700	-0.30908300
C	2.96473000	-0.22903800	1.18166600
H	2.10421200	0.31445000	1.57345900
H	3.48011900	-0.71246600	2.01015000
H	3.65353000	0.49156200	0.74073000
O	-0.08104200	-0.68840200	0.26820100
C	-0.81438800	0.30700100	0.20644000
S	-0.25947600	1.92147300	0.27708200
S	-2.55674600	0.09787600	-0.02984900
C	-2.67207800	-1.69967700	0.02644300
H	-3.73014600	-1.94328700	-0.04679900
H	-2.13404400	-2.14614300	-0.80570400
H	-2.27072000	-2.07412300	0.96471200



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C	-1.51136600	0.66999200	0.94857600
C	-1.00816100	-0.15231200	-0.22570700
C	-1.92714900	-1.31997200	-0.53061100
C	-3.34084500	-0.81414000	-0.81571300
C	-3.87149900	0.02598000	0.34405200

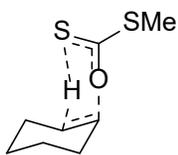
O	0.28480200	-0.71602500	0.08213200
C	1.39269100	-0.01142400	-0.09206400
S	1.51679700	1.50776700	-0.68342800
S	2.72225000	-1.02767500	0.42436200
C	4.13710100	0.03372200	0.12820100
H	4.06154900	0.94198900	0.72063900
H	5.00598000	-0.54622300	0.43508500
H	4.20722100	0.28846800	-0.92611300



TS7-half boat

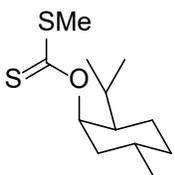
C	1.42720100	0.21285400	1.31166200
C	1.71546600	1.20794700	0.35918800
C	2.14957100	0.80438400	-1.05136900
C	2.64867700	-0.63596900	-1.13413800
C	1.67775600	-1.57309100	-0.42121000
H	0.61665800	1.73201000	0.25122200
H	1.29433500	0.91929500	-1.72319800
H	2.91579500	1.49519800	-1.40320300
H	2.76550600	-0.92488000	-2.17908800
H	3.63499200	-0.71943400	-0.66610900
H	0.67687900	-1.45117600	-0.84917100
H	1.96657300	-2.61599300	-0.55524400
H	2.20469500	2.07979900	0.79375000
O	-0.68637700	-0.04681200	1.25483400
C	-1.28587600	0.49962700	0.32014800
H	1.31078200	0.52153100	2.34306400
C	1.63546200	-1.23691000	1.06338400
H	2.61276800	-1.46053700	1.51823900
H	0.89689400	-1.81918100	1.61287900
S	-1.15239700	2.14886400	-0.08467600
S	-2.30043800	-0.49051200	-0.75123100
C	-2.22035000	-2.07000400	0.11327100

H	-2.87486700	-2.75269800	-0.42518800
H	-1.20473400	-2.46051700	0.11510100
H	-2.56734000	-1.95559200	1.13718800



TS7-half chair

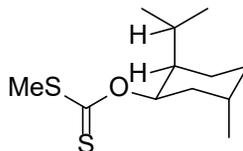
C	1.07951300	-0.86510300	0.92228900
C	1.51167000	0.44951400	1.20565600
C	2.74930200	1.02661600	0.50692900
C	3.50531900	0.00786800	-0.34536800
C	2.53238800	-0.89532800	-1.09785300
H	0.60700800	1.07071600	0.69023600
H	2.42346500	1.85088000	-0.13360400
H	3.41205500	1.45552900	1.25873600
H	4.16527800	0.53116100	-1.03776700
H	4.14188100	-0.61463700	0.29146700
H	1.83745900	-0.28869200	-1.68640000
H	3.06147700	-1.55489400	-1.78577900
H	1.37234200	0.73874600	2.24495000
O	-0.67865100	-0.74148600	-0.19785900
C	-1.33279700	0.31386900	-0.21431000
H	0.45288700	-1.36482500	1.65027500
C	1.73997200	-1.72027500	-0.09494300
H	2.42201500	-2.37307500	0.46994400
H	1.00017400	-2.36794700	-0.56291700
S	-0.66297100	1.86811200	-0.40595700
S	-3.08615400	0.24626700	0.02181800
C	-3.33282700	-1.53685800	0.10932700
H	-4.40614200	-1.69525800	0.19452400
H	-2.95970800	-2.01414300	-0.79321400
H	-2.83021700	-1.95356100	0.97827700



12-a

C	-1.78579800	0.65551500	0.39669100
C	-0.57487100	-0.16075400	0.83655300
C	-0.86996100	-1.65286600	0.89089600
C	-1.44849500	-2.18686400	-0.41969600
C	-2.67093300	-1.36492000	-0.82644600
C	-2.34174000	0.12235200	-0.92548700
H	0.04131100	-2.19011800	1.16235600

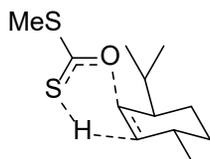
H	-0.21108900	0.19230600	1.80220600
H	-2.53526300	0.44896200	1.17185000
H	-0.68734500	-2.06273200	-1.19819900
H	-3.06003900	-1.73037400	-1.77994900
H	-3.46246900	-1.51809800	-0.08243400
H	-1.60152700	0.27362000	-1.71573600
H	-3.23047700	0.69059800	-1.20975400
H	-1.59107800	-1.81909400	1.69897900
C	-1.53713100	2.17922800	0.41526100
H	-0.83750000	2.37820400	1.23508800
C	-2.83599700	2.92385900	0.72212100
H	-3.24977800	2.62552500	1.68674600
H	-2.67092700	4.00212900	0.74318500
H	-3.58789000	2.72159500	-0.04479800
C	-0.92203800	2.73447200	-0.86990400
H	-0.69230100	3.79338700	-0.74118100
H	-0.00407000	2.21934300	-1.14871300
H	-1.62497900	2.65218700	-1.70184200
C	-1.78279700	-3.66728800	-0.29905200
H	-2.17199800	-4.06073200	-1.23952200
H	-0.90255500	-4.25141000	-0.02544400
H	-2.54284600	-3.82576000	0.47050100
O	0.47551700	0.07447500	-0.13323600
C	1.75226000	-0.01059100	0.20333100
S	2.36924100	-0.35199900	1.67748100
S	2.67247400	0.32810000	-1.24928800
C	4.36098900	0.20817800	-0.65684100
H	4.98953300	0.40910800	-1.52282000
H	4.54358400	0.94504700	0.12102400
H	4.55719700	-0.78903400	-0.27130400



12-e

C	-2.91542900	-1.31027400	-0.73651800
C	-3.41416600	-0.02718500	-0.06512300
C	-2.49990000	0.40997500	1.07774900
C	-1.01601700	0.58605200	0.70179500
C	-0.55646100	-0.66105300	-0.06856900
C	-1.47084800	-1.10681100	-1.20196600
H	-2.87336400	1.32980700	1.52812600
H	-3.48412200	0.76335900	-0.81510700
H	-4.42564500	-0.18230200	0.31920300
H	-3.52218700	-1.48466800	-1.62907400
H	-0.46937100	0.56994000	1.64834800
H	-0.43578200	-1.47712400	0.64722900
H	-1.45296500	-0.36178400	-1.99696300

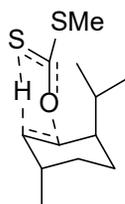
H	-1.07034500	-2.03307400	-1.62079600
H	-2.55248900	-0.34301900	1.86920500
C	-0.60187900	1.93424800	0.06458600
H	0.49157900	1.95227500	0.12889000
C	-0.94895900	2.16303100	-1.40612700
H	-0.63778500	3.16864700	-1.69648100
H	-0.43143300	1.46198100	-2.05883200
H	-2.02148200	2.09045500	-1.59194200
C	-1.11269800	3.10420600	0.90454900
H	-0.94003700	2.94059900	1.97030500
H	-0.60490900	4.02573400	0.61697100
H	-2.18311200	3.26217000	0.75539500
O	0.73465800	-0.44349100	-0.68382900
C	1.84974500	-0.48453100	0.02698000
S	2.00640100	-0.88244300	1.60433900
S	3.14941100	-0.03206500	-1.05732900
C	4.58290900	-0.14511700	0.01427200
H	5.43428000	0.12923300	-0.60646800
H	4.48750600	0.54356200	0.84983600
H	4.69954300	-1.15964300	0.38656400
C	-3.06933600	-2.53680600	0.16232200
H	-4.11394700	-2.67620700	0.44590300
H	-2.73843900	-3.43783500	-0.35689900
H	-2.48752200	-2.45645800	1.08135700



TS8-a

C	2.02428500	0.12080500	0.18463800
C	1.05829600	0.67260800	1.16710700
C	0.20672800	1.75193700	0.90779300
C	0.05727600	2.27996900	-0.51930300
C	1.28395500	1.94900300	-1.36541600
C	1.64217200	0.47034300	-1.25131000
H	-0.88724400	1.26151800	1.22215700
H	1.21188900	0.38772000	2.20291300
H	2.88711600	0.77084300	0.43481500
H	-0.79473200	1.75391200	-0.96657300
H	1.08866400	2.21487000	-2.40633700
H	2.13169800	2.56075400	-1.03429800
H	0.78751200	-0.14159800	-1.55570900
H	2.47127200	0.22152100	-1.91642600
H	0.18361400	2.49115100	1.71185800
C	2.51027100	-1.32974900	0.43633700
H	2.15087700	-1.62669300	1.42436600
C	4.03840200	-1.36998000	0.43938900
H	4.45689200	-0.73913700	1.22603700

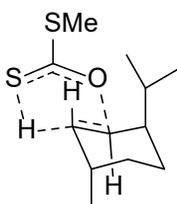
H	4.40089500	-2.38703900	0.59342600
H	4.43184900	-1.01976700	-0.51926500
C	1.97576900	-2.34276800	-0.57337100
H	2.29553900	-3.34483400	-0.28377600
H	0.88981600	-2.33501300	-0.61988000
H	2.37319200	-2.14831800	-1.57205100
C	-0.25757900	3.76910300	-0.51004100
H	-0.41092900	4.14154900	-1.52370500
H	-1.16155400	3.97330900	0.06642900
H	0.56550500	4.33240100	-0.06325800
O	-0.32863700	-1.07819600	1.03811800
C	-1.46645500	-0.82915200	0.63790500
S	-2.47209700	0.38378300	1.31071000
S	-1.97588800	-1.77744700	-0.78658800
C	-3.63577100	-1.17830100	-1.13227200
H	-3.99918900	-1.77818200	-1.96542400
H	-4.28025900	-1.32071700	-0.26828000
H	-3.61965600	-0.12696700	-1.40665100



TS8-e

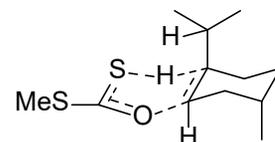
C	1.62111000	-2.22205800	0.10083300
C	2.20658800	-1.20959800	1.08334900
C	2.89503000	-0.06390500	0.35251100
C	1.95823400	0.68024300	-0.61983500
C	0.84187600	-0.15634100	-1.15624000
C	0.60326300	-1.50681600	-0.78626800
H	3.30322900	0.64222800	1.07448800
H	1.39485300	-0.81831000	1.70404200
H	2.91569200	-1.70659400	1.74851900
H	1.07464300	-2.97389200	0.67646000
H	2.51798900	0.87564300	-1.54817900
H	0.40091900	0.20796900	-2.07369500
H	-0.31105500	-1.36358000	-0.05139800
H	0.17569400	-2.10830100	-1.58825900
H	3.75269200	-0.45317900	-0.19887600
C	1.53890200	2.09238300	-0.12356000
H	0.73515800	2.43429000	-0.77583800
C	1.01543200	2.07667100	1.31055100
H	0.58412700	3.04999400	1.54955300
H	0.24385500	1.32267200	1.45798000
H	1.82267200	1.89653700	2.02419800
C	2.71156400	3.06086600	-0.25378200
H	3.03690200	3.16103800	-1.29095200

H	2.42402200	4.04953000	0.10633100
H	3.56846300	2.73360300	0.33964000
O	-0.96138600	0.86948500	-0.54681700
C	-1.90153900	0.24053100	-0.03922400
S	-1.72680400	-0.92973400	1.18986000
S	-3.48523300	0.62632700	-0.75436100
C	-4.63236900	-0.38021100	0.19533100
H	-5.62463000	-0.12201400	-0.17212500
H	-4.43964000	-1.43835300	0.04129900
H	-4.55945700	-0.14668700	1.25482200
C	2.67914800	-2.93929200	-0.73406300
H	3.41912200	-3.42160200	-0.09266900
H	2.22172500	-3.70822400	-1.35841300
H	3.20327700	-2.24896700	-1.39799300



TS9

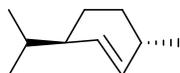
C	-0.87353000	1.78529000	0.47589900
C	-2.40470600	1.93330600	0.18507800
C	-2.95927800	0.99306000	-0.90347700
C	-2.56443700	-0.56531700	-0.78510700
C	-1.13924200	-0.28793300	-0.55576100
C	-0.74401000	0.24559000	0.63922500
H	-4.05099700	1.04243300	-0.92308200
H	-2.94937000	1.77544300	1.11554000
H	-2.60714800	2.96346800	-0.12251200
H	-0.64560600	2.24981200	1.43875800
H	-2.73303600	-0.98649400	-1.77765300
H	-0.56554500	-0.01791400	-1.43832000
H	-1.32631300	-0.08654300	1.49774200
H	0.67517100	0.10311700	0.93762400
H	-2.61657000	1.33068700	-1.88281900
C	-3.36925400	-1.40344900	0.23820600
H	-2.66952100	-2.12171400	0.67531200
C	-4.03938500	-0.64852800	1.38782100
H	-4.62044100	-1.35289600	1.98477400
H	-3.33261700	-0.16300600	2.05660100
H	-4.73250500	0.10885900	1.01551400
C	-4.44092400	-2.19016100	-0.51859500
H	-4.00103700	-2.82800000	-1.28585100
H	-5.01527100	-2.82074300	0.16076000
H	-5.13891900	-1.50551900	-1.00892800
O	1.82237100	-0.12994800	-1.31454000
C	2.60340300	-0.23162900	-0.39985500



TS10

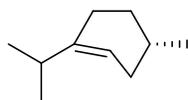
C	3.33693200	-1.29410200	0.21617200
C	3.22478000	-0.26980000	-0.93112800
C	1.78294100	-0.05336200	-1.46818400
C	0.98571300	0.37617300	-0.21047700
C	1.11604300	-0.76263200	0.55492700
C	2.27480600	-1.03438300	1.40622900
H	1.75516600	0.70768200	-2.24867900
H	3.59902600	0.69660200	-0.58367300
H	3.88421700	-0.58579000	-1.74409600
H	4.31059300	-1.15638700	0.69267100
H	-0.34451200	0.32119200	-0.75524500
H	0.72226400	-1.66442000	0.08227200
H	2.62110400	-0.20358400	2.00660700
H	2.20667800	-1.93785300	2.01062300
H	1.38451300	-0.97765200	-1.89081600
C	1.09083500	1.81203600	0.30134300
H	0.06164300	2.02818600	0.61247800
C	1.95127500	2.09871000	1.53395700
H	1.87171100	3.15872700	1.78108700
H	1.60606400	1.53905200	2.40246300
H	3.00834800	1.87966600	1.36396400
C	1.41797100	2.79470600	-0.82136000
H	0.74207400	2.66648000	-1.66825600
H	1.30929900	3.81822900	-0.46153400
H	2.44447400	2.67777700	-1.17934000
O	-1.60954900	0.18520900	1.41989400
C	-2.32810300	0.01255700	0.46742400
S	-1.85447600	0.28387600	-1.20715300
S	-3.98561500	-0.56723100	0.79355600
C	-4.74766000	-0.68943600	-0.83409500
H	-5.76835600	-1.02295500	-0.65220700
H	-4.76709500	0.27770000	-1.33059700
H	-4.23167500	-1.41655100	-1.45550900

C	3.25631300	-2.73168500	-0.29037700
H	4.06798300	-2.92889300	-0.99169700
H	3.34403900	-3.44305600	0.53159100
H	2.31921900	-2.93484500	-0.81029400



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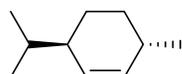
C	-2.11229700	0.48394900	-0.43030100
C	-1.15209400	1.04999200	0.71190300
C	-0.11514800	0.05718100	1.29856700
C	0.71207200	-0.82752000	0.25663300
C	-0.47332200	-1.22001400	-0.57876300
C	-1.03818800	-0.19748100	-1.23640400
H	0.57789300	0.60724200	1.94199600
H	-0.63065500	1.91528300	0.30189900
H	-1.77550600	1.42366600	1.52963000
H	-2.53871800	1.34762300	-0.94334700
H	1.09901400	-1.68188200	0.81711400
H	-1.14369300	-1.87543800	-0.02505500
H	-0.36816600	0.50223700	-1.73011200
H	-0.63937600	-0.64622600	1.95040000
C	1.92044200	-0.13995200	-0.42704600
H	1.94184000	-0.49562200	-1.46123400
C	1.91930800	1.39036500	-0.46080200
H	2.85022900	1.74133200	-0.90949400
H	1.10102400	1.80878500	-1.04242800
H	1.86732400	1.80888600	0.54673300
C	3.20668500	-0.60578100	0.25776600
H	3.30846100	-1.69084700	0.21682900
H	4.08645100	-0.16234700	-0.21100500
H	3.20324400	-0.30840500	1.31050100
C	-3.24854700	-0.39684200	0.10584600
H	-3.33488400	-0.33008900	1.19145200
H	-4.20138900	-0.08142700	-0.31693900
H	-3.11654700	-1.44615900	-0.15132900



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C	-1.68046500	-0.11049600	-0.72696200
C	-1.09272300	1.26646300	-0.29652800
C	-0.26276900	1.31637700	1.06059400
C	0.57702500	0.08673500	0.91503100
C	-0.23840000	-0.99274700	0.90761200
C	-0.71773600	-1.35771700	-0.46118900
H	0.27623200	2.26520500	1.13423900

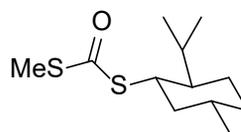
H	-0.44530600	1.62832700	-1.09314300
H	-1.91444400	1.98351900	-0.22452500
H	-1.81920400	-0.06215700	-1.81158100
H	-1.08084200	-0.91002600	1.59353700
H	0.07581800	-1.35832700	-1.20693600
H	-1.29205400	-2.28214200	-0.55160400
H	-0.95170100	1.23597800	1.90308600
C	1.93356400	0.16808500	0.24726900
H	2.54775400	0.70036600	0.98782600
C	2.58350100	-1.19811500	0.03905500
H	3.63228700	-1.07361700	-0.23467500
H	2.52682800	-1.79960400	0.94560700
H	2.10078300	-1.75956500	-0.76146100
C	2.02328400	1.00204100	-1.03743600
H	1.66334900	2.02035000	-0.89159200
H	3.06408100	1.06129700	-1.36019400
H	1.44863300	0.54473000	-1.84591200
C	-3.05681700	-0.34511200	-0.10415900
H	-3.75632600	0.43116300	-0.41723100
H	-3.46664000	-1.30876700	-0.41143300
H	-3.02003600	-0.32980800	0.98628000



ent-8

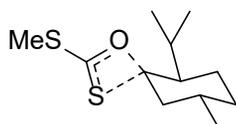
C	-2.11229700	0.48394900	-0.43030100
C	-1.15209400	1.04999200	0.71190300
C	-0.11514800	0.05718100	1.29856700
C	0.71207200	-0.82752000	0.25663300
C	-0.47332200	-1.22001400	-0.57876300
C	-1.03818800	-0.19748100	-1.23640400
H	0.57789300	0.60724200	1.94199600
H	-0.63065500	1.91528300	0.30189900
H	-1.77550600	1.42366600	1.52963000
H	-2.53871800	1.34762300	-0.94334700
H	1.09901400	-1.68188200	0.81711400
H	-1.14369300	-1.87543800	-0.02505500
H	-0.36816600	0.50223700	-1.73011200
H	-0.63937600	-0.64622600	1.95040000
C	1.92044200	-0.13995200	-0.42704600
H	1.94184000	-0.49562200	-1.46123400
C	1.91930800	1.39036500	-0.46080200
H	2.85022900	1.74133200	-0.90949400
H	1.10102400	1.80878500	-1.04242800
H	1.86732400	1.80888600	0.54673300
C	3.20668500	-0.60578100	0.25776600
H	3.30846100	-1.69084700	0.21682900
H	4.08645100	-0.16234700	-0.21100500
H	3.20324400	-0.30840500	1.31050100

C	-3.24854700	-0.39684200	0.10584600
H	-3.33488400	-0.33008900	1.19145200
H	-4.20138900	-0.08142700	-0.31693900
H	-3.11654700	-1.44615900	-0.15132900



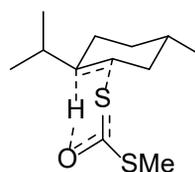
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C	-1.12022400	0.80109000	0.33856700
C	-0.73158800	-0.14867000	-0.80678400
C	-1.09675100	-1.60124000	-0.50239400
C	-2.59347200	-1.75014600	-0.22781400
C	-3.01171000	-0.79722300	0.88757900
C	-2.62863200	0.64700700	0.57822200
H	-0.80527500	-2.23596500	-1.34207400
H	-0.61136700	0.44380000	1.23843500
H	-3.13389400	-1.46031700	-1.13821500
H	-4.08869400	-0.87369800	1.05759300
H	-2.52069600	-1.10961700	1.81662300
H	-3.18155100	0.98510700	-0.30513000
H	-2.93263700	1.28820100	1.40662800
H	-0.53243300	-1.93455800	0.37285000
C	-0.67746800	2.26024600	0.12215700
H	0.41578800	2.25041000	0.09109800
C	-1.08518900	3.14820000	1.29653300
H	-0.83213600	2.68434800	2.25225100
H	-0.57142300	4.10891200	1.24096600
H	-2.15776100	3.35156600	1.29184800
C	-1.16763500	2.86324000	-1.19261500
H	-0.85048000	3.90454500	-1.26895200
H	-0.76646600	2.33842400	-2.06089600
H	-2.25808500	2.84882400	-1.25511700
C	-2.94417100	-3.19403100	0.10499700
H	-4.01536900	-3.30844700	0.27943200
H	-2.65783800	-3.86894500	-0.70334700
H	-2.42067300	-3.51282500	1.00961000
H	-1.27871900	0.15789000	-1.70599500
S	0.98908700	0.00147300	-1.40403100
C	1.94356000	-0.39212400	0.03049200
O	1.50916000	-0.69655100	1.10684900
S	3.68266100	-0.27496500	-0.31898000
C	4.29537500	-0.76080600	1.30290300
H	3.95764600	-1.76457400	1.54580400
H	5.38093300	-0.73538100	1.23977100
H	3.94732500	-0.06268300	2.05915000



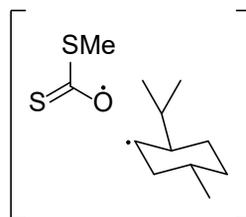
TS11

C	-2.28072300	0.02674600	-0.57046200
C	-0.84830200	-0.01584200	-0.62668000
C	-0.08303500	1.12545800	-1.08685000
C	-0.22113700	2.19060600	0.07678800
C	-1.69428700	2.33209800	0.43512300
C	-2.31314700	0.97630500	0.72863900
H	0.97039500	0.88711300	-1.22143400
H	-0.34008100	-0.82995700	-0.12557500
H	-2.72529500	0.61795400	-1.37480900
H	0.31800600	1.77155000	0.92896400
H	-1.78860200	2.96843000	1.31831100
H	-2.23397400	2.82848100	-0.37817800
H	-1.78719100	0.49033600	1.55237200
H	-3.37114700	1.03683000	0.98750100
H	-0.51563400	1.56970000	-1.98656800
C	-3.00416700	-1.31393300	-0.37111100
H	-2.72140800	-1.93329600	-1.22746700
C	-4.51664300	-1.11915200	-0.41585200
H	-4.83185800	-0.61319400	-1.33018300
H	-5.02013600	-2.08512100	-0.37683100
H	-4.86969000	-0.53609300	0.43736000
C	-2.57908400	-2.04658700	0.89937400
H	-3.01172400	-3.04704700	0.90242300
H	-1.49614900	-2.15728400	0.98342000
H	-2.94283400	-1.52999100	1.78978700
C	0.43298600	3.48981000	-0.35917700
H	0.38383300	4.22197800	0.44811900
H	1.48293100	3.32780200	-0.60302700
H	-0.06964200	3.90983200	-1.23325600
O	0.98065300	-0.43916000	1.40162300
C	1.81138300	-0.82838000	0.58092900
S	1.59636900	-2.08182200	-0.55853400
S	3.31949800	0.16696500	0.58528900
C	4.35498500	-0.58092100	-0.68225600
H	5.29069300	-0.02269600	-0.67814900
H	4.54446300	-1.62481700	-0.44541900
H	3.88296600	-0.51677700	-1.65922100

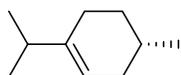


TS12

C	1.43074200	-0.14790200	0.09891200	H	-1.83458700	-1.25798400	1.87648600
C	0.90540000	0.30083500	-1.12144300	H	-3.28211000	0.33242700	0.67547100
C	0.10505500	1.56716300	-1.24959300	H	0.21259900	1.94884800	-1.29688200
C	0.45853200	2.59831000	-0.17466400	H	-1.89357800	2.20279400	0.26807600
C	0.41495600	1.91069100	1.18461800	H	-2.22228500	1.56797500	-1.32621000
C	1.47123800	0.81849200	1.28649400	H	-0.05349500	-1.72954000	0.30240500
H	0.23663800	1.97195900	-2.25527200	C	2.02757900	0.22186000	-0.41072500
H	0.41400400	-0.82680300	0.43404300	H	2.21347600	0.93275800	-1.22058900
H	1.48252600	2.95112000	-0.34630100	C	2.87225900	0.65328400	0.79124700
H	0.55868100	2.63967600	1.98528400	H	3.93232900	0.65781500	0.53073300
H	-0.58247800	1.47455600	1.32138100	H	2.59517600	1.65398900	1.12409200
H	2.46523200	1.27740100	1.32953500	H	2.74393300	-0.03260900	1.63099400
H	1.34440800	0.25966700	2.21505300	C	2.45284100	-1.16719300	-0.88999200
H	-0.96088200	1.33879200	-1.15517500	H	1.84699300	-1.49580800	-1.73614900
C	2.53376100	-1.20552900	0.01078000	H	3.49929700	-1.16162400	-1.19894100
H	2.20695300	-1.91998300	-0.75253400	H	2.34857700	-1.90469400	-0.09117100
C	2.70210600	-1.96542200	1.32373900	C	-2.53102100	-1.00460000	-0.81350000
H	1.75115400	-2.37345700	1.66993300	H	-2.86216100	-1.93907900	-0.35576500
H	3.40169700	-2.79213500	1.19543700	H	-3.28884300	-0.69449700	-1.53462800
H	3.10220500	-1.31505300	2.10484900	H	-1.61108500	-1.20403300	-1.36688600
C	3.86281400	-0.59533200	-0.43527300				
H	4.62453800	-1.36906400	-0.54412500				
H	3.76435700	-0.08085500	-1.39292600				
H	4.22782900	0.12456500	0.30071700				
C	-0.49253700	3.78385800	-0.24632000				
H	-0.22884000	4.54430400	0.49001100				
H	-0.47739400	4.24773200	-1.23404100				
H	-1.51611600	3.45721700	-0.04523900				
H	1.30565000	-0.12440000	-2.03253000				
S	-0.90474300	-1.44524300	-1.80658000				
C	-1.46285500	-1.23434200	-0.23119200	C	3.98799300	-0.81280300	0.68534400
O	-0.74900400	-1.42693400	0.78350500	C	3.40893400	0.48690500	1.24754800
S	-3.07575200	-0.54790300	-0.02280200	C	2.82323800	1.38496000	0.15566800
C	-3.20999100	-0.57302400	1.77508300	C	1.80691000	0.68985800	-0.77373700
H	-3.08599600	-1.58807000	2.14406100	C	2.10966000	-0.76137000	-0.97988300
H	-2.46198000	0.07235300	2.22792100	C	2.85938400	-1.59547300	0.00329800
H	-4.20755700	-0.21049400	2.01515500	H	2.36493400	2.26370100	0.61445600
				H	2.64021300	0.23230500	1.98196700
				H	4.18632100	1.03775200	1.78388800
				H	4.35985800	-1.40907800	1.52315800
				H	1.87894300	1.17381700	-1.75542900
				H	1.59486300	-1.25837700	-1.79382500
				H	2.17981900	-1.96653100	0.78714600
				H	3.25786100	-2.48643500	-0.49010200
				H	3.64709500	1.76499700	-0.45231800
				C	0.32293200	0.89688700	-0.35621600
				H	-0.25951300	0.26015400	-1.02864900
				C	0.03482600	0.46209300	1.07675600
				H	-1.03298000	0.55799000	1.28982200
				H	0.32551900	-0.57505200	1.25362400
				H	0.56296100	1.09782700	1.79164200



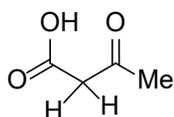
Int1



ent-7

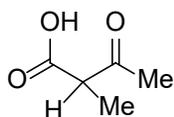
C	-2.31187700	0.07868800	0.24052600	H	1.59486300	-1.25837700	-1.79382500
C	-1.39059600	-0.40174000	1.36342900	H	2.17981900	-1.96653100	0.78714600
C	-0.00869600	-0.77035300	0.83060700	H	3.25786100	-2.48643500	-0.49010200
C	0.54809800	0.27760000	-0.10106400	H	3.64709500	1.76499700	-0.45231800
C	-0.23506400	1.21333000	-0.63377700	C	0.32293200	0.89688700	-0.35621600
C	-1.71319600	1.34132800	-0.38456200	H	-0.25951300	0.26015400	-1.02864900
H	0.68060100	-0.92888900	1.66433800	C	0.03482600	0.46209300	1.07675600
H	-1.28679800	0.39892400	2.10147900	H	-1.03298000	0.55799000	1.28982200
				H	0.32551900	-0.57505200	1.25362400
				H	0.56296100	1.09782700	1.79164200

C	-0.14228200	2.33276300	-0.57837000
H	0.02256700	2.64556900	-1.61049600
H	-1.21067500	2.42081300	-0.37019400
H	0.38146200	3.03131300	0.07826400
C	5.15015300	-0.56892900	-0.27414200
H	5.91167500	0.06681200	0.18226300
H	5.62114900	-1.51240200	-0.55526200
H	4.81151200	-0.08618300	-1.19289600
O	-2.68722300	0.32584900	-1.85054500
C	-2.95587500	-0.18592600	-0.80185200
S	-2.39320100	-1.82749400	-0.46414300
S	-3.90424900	0.66362300	0.42228100
C	-3.92834300	-0.50923900	1.79289400
H	-4.49047600	-0.01664200	2.58413000
H	-4.44012900	-1.42921500	1.51807400
H	-2.92116300	-0.71632700	2.15104600



16a

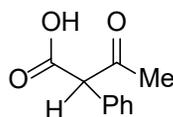
C	1.19910000	0.09448800	0.04426800
C	2.48137600	-0.64845900	-0.18707400
H	3.31432000	0.04680200	-0.23906400
H	2.64008800	-1.38141200	0.60581900
H	2.40213900	-1.20361700	-1.12466300
O	1.14780300	1.30369700	0.01128400
C	-0.02197600	-0.74574800	0.35185400
H	0.05592400	-1.73704000	-0.09013100
H	-0.02356000	-0.89232900	1.43878600
C	-1.39245300	-0.17385600	-0.00749800
O	-1.49867800	1.15026300	-0.03236400
H	-0.61186300	1.55301500	0.06209900
O	-2.32079200	-0.89695700	-0.21168800



16b

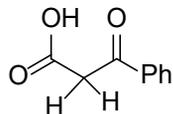
C	-1.20018200	-0.27512100	-0.07599500
C	-2.45266100	0.22510500	-0.73325500
H	-3.30235200	-0.38520300	-0.44085000
H	-2.62399800	1.27232600	-0.47874600
H	-2.31823400	0.17750600	-1.81662600
O	-1.17423300	-1.32124900	0.53479300
C	0.02199700	0.61658600	-0.17240900
C	1.36387700	-0.10625200	-0.29414200

O	1.47617500	-1.27329900	0.33514400
H	0.59810800	-1.55404100	0.66206300
O	2.27962600	0.39682300	-0.87520100
C	0.06790700	1.48922500	1.09879700
H	0.91264400	2.17275900	1.03600000
H	-0.84709900	2.07283500	1.20248100
H	0.18275300	0.86231500	1.98297100
H	-0.05998900	1.26603900	-1.04315400



16c

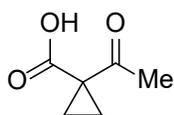
C	-1.55740300	1.16863700	-0.11704600
C	-1.46412100	2.36242400	-1.01947300
H	-1.79996400	3.25456600	-0.49869800
H	-0.43856600	2.48276500	-1.37259500
H	-2.09313900	2.18845800	-1.89581600
O	-2.11361800	1.21914400	0.95837300
C	-0.87132700	-0.09395200	-0.60949300
H	-0.94215000	-0.13818600	-1.69575000
C	-1.43084200	-1.42762300	-0.09433500
O	-1.99248800	-1.42025500	1.11039700
H	-2.11338100	-0.49536900	1.40721600
O	-1.31147700	-2.42305200	-0.74341200
C	0.60536200	-0.00809400	-0.23823200
C	1.57374100	-0.27585500	-1.19957700
C	0.99722500	0.30433200	1.06024600
C	2.91985800	-0.22792500	-0.86823700
H	1.26995600	-0.53731500	-2.20564100
C	2.34400800	0.35206900	1.38928400
H	0.25083000	0.50897000	1.81861400
C	3.30755500	0.08792000	0.42620300
H	3.66573800	-0.44177000	-1.62246900
H	2.63942600	0.59447000	2.40158900
H	4.35757600	0.12511700	0.68464800



16d

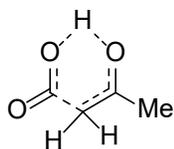
C	-0.47889200	-0.46954500	-0.00005600
O	-0.83646700	-1.63162700	-0.00005000
C	-1.47719600	0.66736800	-0.00015700
H	-1.29218400	1.30394000	0.86797600
H	-1.29234900	1.30352400	-0.86864500
C	-2.97558200	0.35664500	0.00005200

O	-3.34673300	-0.91540600	-0.00010500
H	-2.54817100	-1.48539700	-0.00014400
O	-3.76259000	1.25668500	0.00028800
C	0.97167900	-0.13269200	-0.00001400
C	1.43013500	1.18351300	-0.00009100
C	1.88951800	-1.18320100	0.00009200
C	2.79180700	1.44504500	-0.00005900
H	0.73410600	2.01163000	-0.00017600
C	3.24724700	-0.91972300	0.00012300
H	1.51618600	-2.19845200	0.00015000
C	3.69907200	0.39513700	0.00004600
H	3.14395800	2.46781900	-0.00011700
H	3.95642700	-1.73670200	0.00020700
H	4.76162200	0.60114000	0.00007300



16e

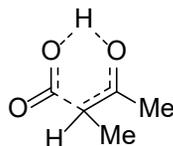
C	1.18137100	0.53385400	0.01682800
C	2.54106400	-0.10065000	-0.12612400
H	3.28206300	0.57000000	0.30037100
H	2.61420200	-1.08586200	0.32834200
H	2.74875300	-0.20830500	-1.19346200
O	1.10079500	1.74524100	0.10300600
C	-0.03313500	-0.32314800	0.00891300
C	-1.41484200	0.29821200	-0.04540300
O	-1.48324000	1.61899900	-0.00719500
H	-0.57349300	1.98735400	0.05922400
O	-2.39315000	-0.39256300	-0.11256700
C	0.00782100	-1.61753400	0.82378300
H	-0.92928600	-1.85134900	1.30692900
H	0.90190900	-1.80832400	1.39828900
C	0.05480300	-1.69652800	-0.64250000
H	0.98717400	-1.94904800	-1.12512300
H	-0.84906100	-1.99313000	-1.15349900



TS13a

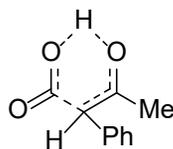
C	1.11496800	-0.01303800	0.18265300
C	0.04711700	-0.68245400	0.79802100
H	0.07312500	-1.76214400	0.79528900
H	-0.31096700	-0.23922400	1.72318900
O	1.08062100	1.27045000	0.07053400
C	2.27627200	-0.69375700	-0.44721200

H	2.10305400	-1.76171300	-0.54596800
H	2.49745900	-0.24203400	-1.41310500
H	3.14585300	-0.53959700	0.19715000
H	0.06925000	1.51434900	0.11049300
O	-1.35206400	1.15737600	-0.16407500
C	-1.43741700	-0.06491300	-0.09511000
O	-2.17648300	-0.95840900	-0.34360400



TS13b

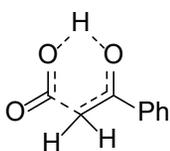
C	1.15263900	0.00646600	0.00211400
C	0.03868400	0.62423200	0.59805800
H	0.05980900	0.62143000	1.68107000
O	1.16493900	-0.18337500	-1.27521300
C	2.30176000	-0.55140900	0.76176500
H	2.06252700	-0.65163600	1.81731500
H	2.61102400	-1.50489400	0.33730800
H	3.13920400	0.14549100	0.66444300
H	0.15754300	-0.26749100	-1.53179000
O	-1.22312400	-0.68995000	-1.13339800
C	-1.27854200	-0.54211600	0.08550100
O	-1.95755500	-0.83630700	1.01663900
C	-0.52950300	1.90442600	-0.00937000
H	-0.51279300	1.87124900	-1.09652800
H	-1.55938500	2.05216800	0.31268100
H	0.05776300	2.76114400	0.32287200



TS13c

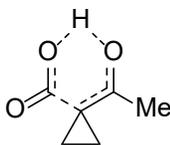
C	1.80931300	-0.81206200	-0.33868400
C	0.80048100	0.11167900	-0.68780800
H	0.93997900	0.54865000	-1.66944200
O	1.90504900	-1.22988000	0.87238100
C	2.85077400	-1.27179000	-1.29462400
H	3.03948500	-0.51139000	-2.05017700
H	3.76510700	-1.53749300	-0.76955000
H	2.47065900	-2.15929700	-1.80881600
H	1.49713300	-0.43699300	1.45069400
O	1.24799700	0.95981200	1.65665200
C	1.13510200	1.46454400	0.54224100
O	1.09684100	2.52041300	0.00381900
C	-0.64902700	-0.10909300	-0.36343400

C	-1.57497600	0.71873500	-0.99730400
C	-1.11037300	-1.08535600	0.51660300
C	-2.93251700	0.56954800	-0.76449500
H	-1.22057000	1.49176200	-1.66832100
C	-2.47102800	-1.23468300	0.74291300
H	-0.41732500	-1.74059900	1.02650800
C	-3.38728100	-0.41005300	0.10691800
H	-3.63553700	1.22325500	-1.26407000
H	-2.81403200	-2.00166900	1.42511300
H	-4.44680300	-0.52780000	0.29128300



TS13d

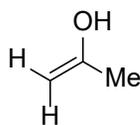
C	0.55219000	0.30944800	-0.63239300
C	1.49779100	-0.71079500	-0.81361600
H	1.18186100	-1.73201100	-0.67089500
H	2.19255500	-0.55763200	-1.63428400
O	0.95173900	1.54349800	-0.68533100
H	1.94866800	1.51506800	-0.43035200
O	3.08945800	0.86452000	0.33724700
C	2.81958600	-0.32567900	0.42900500
O	3.15474900	-1.32037700	0.98117000
C	-0.85241700	0.09865900	-0.26873300
C	-1.46885600	-1.13834400	-0.46435600
C	-1.58521400	1.15951600	0.26884200
C	-2.79657100	-1.31432300	-0.11546700
H	-0.91774000	-1.95651600	-0.90693600
C	-2.91149000	0.97790700	0.61784500
H	-1.09890800	2.11397400	0.41429600
C	-3.51697200	-0.25826800	0.42777500
H	-3.27218800	-2.27316900	-0.27127400
H	-3.47514400	1.79865800	1.04066200
H	-4.55494800	-0.39822600	0.70068300



TS13e

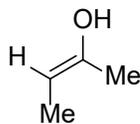
C	-1.21764500	-0.21651300	0.03133500
O	-1.32271800	-1.36415100	0.64233200
H	-0.39491200	-1.66443300	0.85856200
O	1.15649700	-1.70883200	0.24643300
C	1.36053400	-0.66166800	-0.32484100
O	2.13288100	-0.05555700	-0.99024400

C	-0.05504600	0.52236200	0.10989400
C	0.18710800	1.95366000	-0.12265700
C	0.57517400	1.33444900	1.19858300
H	-0.65553300	2.63357500	-0.12797000
H	0.99841600	2.19761400	-0.79625800
H	1.62867100	1.19853800	1.40206400
H	-0.03662600	1.55351800	2.06344500
C	-2.38420000	0.14146000	-0.81823100
H	-3.22453000	0.38381600	-0.16216700
H	-2.16332700	0.99826100	-1.44715800
H	-2.68099200	-0.71506800	-1.42318600



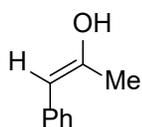
Int2a

C	-0.08317800	-0.05059000	0.00000000
C	-0.97321700	-1.03727300	0.00000000
H	-0.64655800	-2.06527800	0.00000200
H	-2.03849600	-0.84284000	0.00000000
O	-0.41405900	1.27150600	-0.00000200
C	1.39816200	-0.22331600	0.00000100
H	1.66598000	-1.27666600	0.00000300
H	1.82685000	0.25893600	-0.87984700
H	1.82684800	0.25893900	0.87984900
H	-1.37276000	1.36193400	-0.00000500



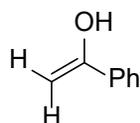
Int2b

C	0.46426100	-0.01656700	0.00000000
C	-0.65243700	-0.74016800	0.00000000
H	-0.55384900	-1.81627000	0.00000100
O	0.46780700	1.34919200	0.00000000
C	1.85330800	-0.55604800	0.00000000
H	1.84415100	-1.64333700	-0.00000100
H	2.39257800	-0.20109600	-0.87996700
H	2.39257800	-0.20109800	0.87996800
H	-0.43838800	1.67543000	0.00000300
C	-2.02799300	-0.13371300	0.00000000
H	-2.79482200	-0.90545300	-0.00001400
H	-2.20377400	0.48862000	0.88344700
H	-2.20376400	0.48864000	-0.88343600



Int2c

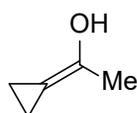
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C	-1.09488900	-0.73395500	-0.37559300
H	-1.30760700	-1.69924600	-0.81587200
O	-2.04405600	1.17870000	0.68975600
C	-3.56640400	-0.40563300	-0.14024600
H	-3.64487600	-1.35413100	-0.66535200
H	-4.05211600	-0.48681200	0.83354900
H	-4.09635200	0.36268100	-0.70620700
H	-1.11964900	1.35530600	0.90650200
C	0.31921500	-0.36107500	-0.21510600
C	1.25670900	-1.32837300	0.15965700
C	0.77778600	0.93982700	-0.44820500
C	2.59328400	-1.00424600	0.32144700
H	0.92167700	-2.34439400	0.33055000
C	2.11653400	1.26691300	-0.27858700
H	0.08667900	1.69254000	-0.81039000
C	3.02905200	0.29852000	0.11157200
H	3.29962000	-1.77028400	0.61506500
H	2.44823300	2.27962900	-0.46908600
H	4.07300700	0.55219000	0.23985600



Int2d

C	-1.68952300	0.05616200	0.00233100
C	-2.43912800	1.11765200	0.29431400
H	-1.98940600	2.05492100	0.57845200
H	-3.51998200	1.06400300	0.27369000

O	-2.21523200	-1.16404900	-0.30298200
H	-3.17256900	-1.12713900	-0.21171000
C	-0.21101600	0.03769400	-0.00806000
C	0.52406100	1.21350500	-0.15738900
C	0.46942300	-1.16985100	0.13668800
C	1.90813700	1.18448900	-0.13972600
H	0.00969200	2.15279300	-0.31136000
C	1.85637100	-1.19648800	0.15438800
H	-0.09634800	-2.08513800	0.23889400
C	2.58009000	-0.02112700	0.01984900
H	2.46546400	2.10420300	-0.26143800
H	2.37247000	-2.14046400	0.27261000
H	3.66204700	-0.04299800	0.03034100



Int2e

C	0.77141100	-0.06217400	0.00012800
O	1.43197900	-1.25968500	-0.00000800
C	1.71629100	1.08990600	-0.00008900
H	1.16931500	2.02936100	0.00034700
H	2.36028500	1.04435900	0.87990300
H	2.35941300	1.04474800	-0.88075100
H	0.77805600	-1.96775700	0.00008300
C	-0.54252500	0.02837700	0.00030100
C	-1.82925200	-0.66912800	-0.00014700
C	-1.73786800	0.85873200	0.00005700
H	-2.17263700	-1.14330200	0.91190500
H	-2.17215500	-1.14283700	-0.91262400
H	-2.02289500	1.36914200	-0.91221100
H	-2.02355600	1.36948500	0.91191100

3. Source Data of Distances of Key Bonds and Mayer Bond Order in Transition States

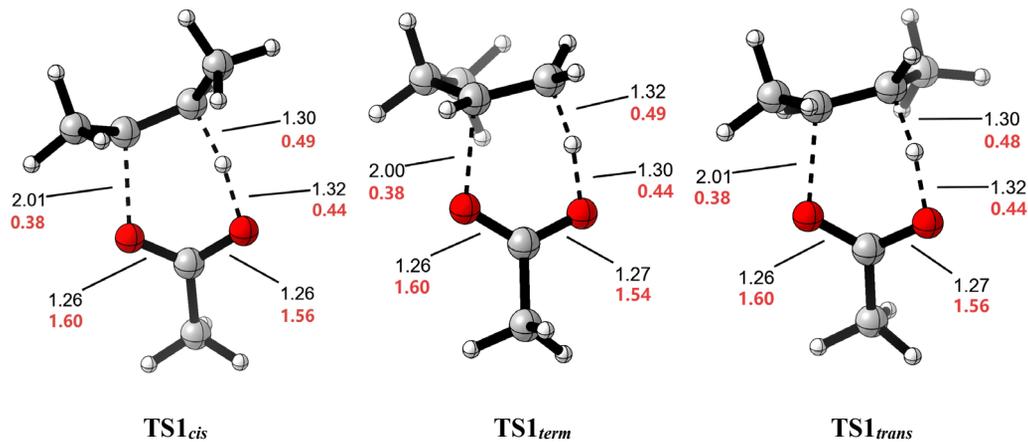


Figure S1. Distances of key bonds and Mayer bond order in transition states TS1s

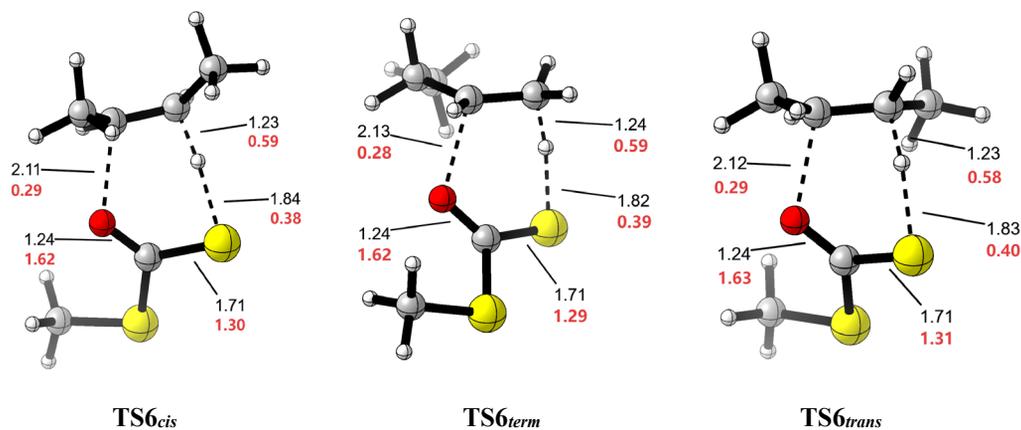
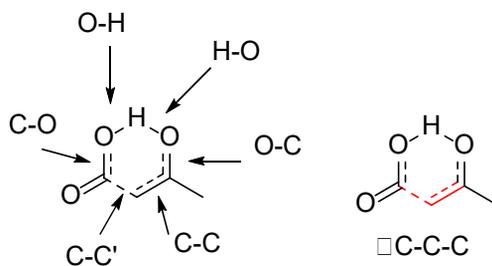


Figure S2. Distances of key bonds and Mayer bond order in transition states TS6s

Table S1. Distances of key bonds and key angles in transition states TS14s



Structure	O-C Å	C-C Å	C-C' Å	C-O Å	O-H Å	H-O Å	∠C-C-C	ΔΔG kcal/mol
TS13a	1.29	1.40	1.84	1.23	1.49	1.04	104°	23.4
TS13b	1.29	1.41	1.83	1.23	1.50	1.04	103°	24.8
TS13c	1.29	1.41	1.86	1.23	1.43	1.06	100.6°	24.2
TS13e	1.30	1.38	1.9	1.21	1.67	1.00	106.4°	32.8
TS13d	1.30	1.4	1.85	1.22	1.52	1.03	104.1°	23.2

4. Computed Energies

Table S2. Electronic energies under M06-2X/def2-tzvp (E_{gas} in Hartree), thermal corrections to Gibbs free energies under M06-2X/def2-tzvp ($\Delta G_{correction}$ in Hartree). The contribution of vibration to entropy was calculated using a quasi-rigid-rotor-harmonic-oscillator (quasi-RRHO) approximation, which uses the Grimme method implemented in the Shermo program, switching to a free rotor description of vibrational modes below 100 cm^{-1} . The relative Gibbs free energies were corrected with quasi-RRHO and the scale factor of 0.971 was employed for ZPE (G_{shermo} in Hartree).

Structure	E_{gas}	$\Delta G_{correction}$	G_{gas}	temperature	G_{shermo}	ΔG_{gas} (kcal/mol)	ΔG_{shermo} (kcal/mol)
1	-386.3178534	0.140523	-386.1773304	450°C	-386.2597183	0.0	0.0
TS1 _{cis}	-386.2328218	0.132332	-386.1004898	450°C	-386.1823521	48.2	48.5
TS1 _{trans}	-386.2337745	0.132409	-386.1013655	450°C	-386.1836043	47.7	47.8
TS1 _{term}	-386.2342315	0.133147	-386.1010845	450°C	-386.1820722	47.8	48.7
cis-But-2-ene	-157.1963979	0.080799	-157.1155989	450°C	-157.1744319	3.8	-15.2
trans-But-2-ene	-157.1981165	0.081179	-157.1169375	450°C	-157.1756815	2.9	-16
But-1-ene	-157.1935642	0.081664	-157.1119002	450°C	-157.1713956	6.1	-13.3
cis-2	-542.3572304	0.231854	-542.1253764	450°C	-542.2264624	0.0	0.0
TS2 _{cis-less}	-542.2772012	0.222436	-542.0547652	450°C	-542.1559326	44.3	44.3
TS2 _{cis-term}	-542.2816034	0.222347	-542.0592564	450°C	-542.1591143	41.5	42.3
3	-313.2395097	0.171686	-313.0678237	450°C	-313.1479462	1.2	-19.5
4	-313.2376837	0.172785	-313.0648987	450°C	-313.1441417	3.0	-17.1
trans-2	-542.3550586	0.23229	-542.1227686	450°C	-542.2236176	0.0	0
TS2 _{trans-more}	-542.2759413	0.222099	-542.0538423	450°C	-542.1548598	43.3	43.1
TS2 _{trans-less}	-542.2748597	0.222317	-542.0525427	450°C	-542.1530122	44.1	44.3
TS2 _{trans-term}	-542.2829084	0.223513	-542.0593954	450°C	-542.1592956	39.8	40.4
3	-313.2395097	0.171686	-313.0678237	450°C	-313.1479462	-0.5	-21.3
4	-313.2376837	0.172785	-313.0648987	450°C	-313.1441417	1.4	-18.9
5	-313.2406641	0.170103	-313.0705611	450°C	-313.1505905	-2.2	-22.9
AcOH	-229.09103	0.035328	-229.055702	450°C	-229.1095654		
6	-620.9744956	0.284372	-620.6901236	450°C	-620.8028146	0.0	0.0
TS3	-620.8874444	0.276804	-620.6106404	450°C	-620.7238067	49.9	49.6
TS4	-620.8836596	0.277403	-620.6062566	450°C	-620.7180858	52.6	53.2
TS5	-620.8531462	0.276396	-620.5767502	450°C	-620.6903131	71.1	70.6
7	-391.8572248	0.224319	-391.6329058	450°C	-391.7261955	1.0	-20.6
8	-391.8533706	0.224721	-391.6286496	450°C	-391.7213601	3.6	-17.6
9	-391.7685871	0.223686	-391.5449011	450°C	-391.6383404	56.2	34.5
10	-1107.443887	0.136436	-1107.307451	350°C	-1107.374414	0.0	0.0
TS6 _{cis}	-1107.372683	0.127459	-1107.245224	350°C	-1107.312509	39.0	38.8

TS6_{trans}	-1107.373794	0.127445	-1107.246349	350°C	-1107.313683	38.3	38.1
TS6_{term}	-1107.372145	0.127734	-1107.244411	350°C	-1107.310903	39.6	39.9
MeSCOSH	-950.2204402	0.026385	-950.1940552	350°C	-950.222349		
cis-But-2-ene	-157.1963979	0.080799	-157.1155989	350°C	-157.1596607	-1.4	-4.8
trans-But-2-ene	-157.1981165	0.081179	-157.1169375	350°C	-157.1609353	-2.2	-5.6
But-1-ene	-157.1935642	0.081664	-157.1119002	350°C	-157.1566279	0.9	-2.9
11	-1184.864743	0.174497	-1184.690246	-	-		0
TS7-half chair	-1184.792233	0.165604	-1184.626629	-	-		39.9
TS7-half boat	-1184.792448	0.166764	-1184.625684	-	-		40.5
MeSCSOH	-950.2204402	0.026385	-950.1940552	220°C	-950.222349		
Int1	-1341.985763	0.268565	-1341.717198	220°C	-1341.769574	63.1	62.9
12-a	-1342.098675	0.28088	-1341.817795	220°C	-1341.869854	0.0	0.0
12-e	-1342.089752	0.282331	-1341.807421	220°C	-1341.859335	6.5	6.6
TS8-a	-1342.0236	0.27211	-1341.75149	220°C	-1341.803236	41.6	41.8
TS8-e	-1342.021383	0.275264	-1341.746119	220°C	-1341.79823	45.0	44.9
TS9	-1341.974108	0.268483	-1341.705625	220°C	-1341.757932	70.4	70.2
TS10	-1341.968916	0.268226	-1341.70069	220°C	-1341.752401	73.5	73.7
ent-8	-391.8533706	0.224721	-391.6286496	220°C	-391.6673847	-1.6	-12.5
13	-391.7525017	0.224658	-391.5278437	220°C	-391.5683174	60.2	49.7
14	-391.7601881	0.22458	-391.5356081	220°C	-391.5772284	55.3	44.1
TS11	-1342.00787	0.274006	-1341.733864	220°C	-1341.786282	52.7	52.4
15	-1342.113638	0.278531	-1341.835107	220°C	-1341.887767	-10.9	-11.2
TS12	-1342.030627	0.271392	-1341.759235	220°C	-1341.811697	36.7	36.5
ent-7	-391.856165	0.224765	-391.6314	220°C	-391.67288	-4.8	-15.9
16a	-381.7294572	0.06844	-381.6610172	-	-		0
16b	-421.0384323	0.095921	-420.9425113	-	-		0
16c	-612.7682698	0.143376	-612.6248938	-	-		0
16d	-573.4617514	0.117142	-573.3446094	-	-		0
16e	-459.1249719	0.102648	-459.0223239	-	-		0
TS13a	-381.6892824	0.065533	-381.6237494	-	-		23.4
TS13b	-420.9954812	0.092455	-420.9030262	-	-		24.8
TS13c	-612.726516	0.140222	-612.586294	-	-		24.2
TS13d	-573.423269	0.115566	-573.307703	-	-		23.2
TS13e	-459.0680621	0.098017	-458.9700451	-	-		32.8
Int2a	-193.1255688	0.058679	-193.0668898	-	-		-7.2
Int2b	-232.4349439	0.083499	-232.3514449	-	-		-9.1
Int2c	-424.1714427	0.133727	-424.0377157	-	-		-11.6
Int2d	-384.8561762	0.107029	-384.7491472	-	-		-6.4
Int2e	-270.4962914	0.089576	-270.4067154	-	-		6.3

Note: The thermal correction of Gibbs free energies was conducted for the temperatures at which

corresponding eliminations were carried out. Crucially, the high-temperature correction significantly increases the exothermicity (due to the large entropy contribution in elimination reactions), rendering the reactions thermodynamically feasible. Without this correction, the Gibbs free energies of some products would theoretically exceed those of the reactants, implying non-spontaneity. Regarding the relative energy order, we have included a comparison of energies before and after temperature correction in the Table S2. This analysis reveals that the correction does influence the relative stabilities within specific groups, notably the **TS1_{cis}/TS1_{trans}/TS1_{term}** group and the products **7/15** group. For other species, the correction results in a uniform energy shift without altering their relative rankings or the associated conclusions.