Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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ELECTRONIC SUPPLEMENTARY INFORMATION for:

"Unraveling the stereoselectivity in 6-*exo*-trig radical cyclization of *α,β*-unsaturated ester-tethered sugars. A tale of two stereocenters"

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1. Experimental Details

All isolated structures were computed using DFT UB3LYP[1] as implemented in the GAMESS[2] suite of programs. A mixed basis set was employed throughout for geometry optimizations and frequency analyses of all species. We denote this mixed basis set as MIX and it comprises 6-31G(d,p) for the atoms at the reaction center and nearby, and 3-21G(d,p) for the atoms at the periphery (see Figure 1 for partitioning). Further single-point using 6-31G(d,p) basis set was computed to get more accurate results. For the TS structures, we also checked single points with and 6-311++G(2d,2p). The geometry of all ground state structures was fully optimized and in the case of transition states, a "loose" geometry convergence criterion was set to rms gradient below 0.0005 hartree/au. Tests showed that further optimization did not result in significant improvements in the geometry or energy. Spin contamination ($<S^2>$) values never exceeded 0.79, which is close to the theoretical expected value of 0.75. All species were verified by vibrational frequency analysis in order to ascertain that the computed transition states represented first-order saddle points. The total energies were corrected by zero-point vibrational energy (ZPE) and the respective thermal contributions at 353 K. Translational, rotational and vibrational entropies were also included.

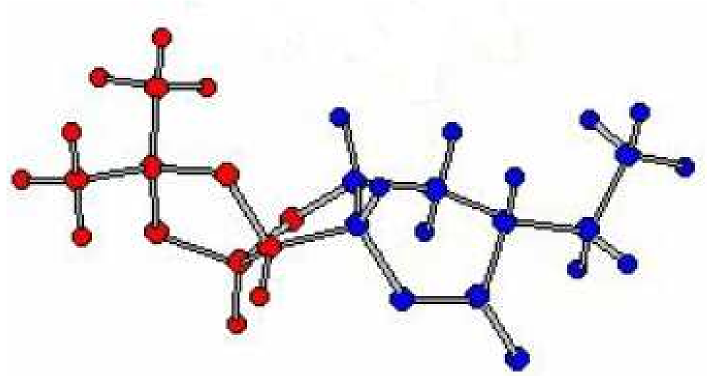

FIGURE 1. MIX: blue region was modeled with **6-31G(d,p)**, while red region was modeled with **3-21G(d,p)**.

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(1) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

(2) Schmidt, M. W.; Baldridge, K. K.; Boatz, J. A.; Elderbert, S. T.; Gordon, M. S.; Jensen, J. H.; Kosek, J.; Matsunaga, N.; Nguyen, K. A.; Su, S. J.; Windus, T. L.; Dupius, M.; Montgomery, J. A. *J. Comp. Chem.* **1993**, *14*, 1347.

2. TS mimic models for lactone 2

To further test the ester-controlled boatlike TS model, we tackled a second sugar (lactone **2**) and applied the same rationality as depicted on Figure 2 (see article). All attempts were made to reproduce closely the TS structures of lactone **1**, but bearing in mind the differences between the systems (mainly the *trans*-junction at the carbohydrate moiety**)**. From lactone **1**, we followed two rules: (1) the distance of attack of the radical to the *exo* carbon was set to 2.30 Å and (2) the trend of ϕ_1 values. MM+ force field available at Hyperchem 6.0[3] was used to build the models. Benzyl groups were replaced by methyl groups to improve visualization. A similar boatlike **TS1-pyranose** was produced with the ester in a nearly planar conformation to account for the only stereoisomer isolated in the reaction. The attempt to produce a second boatlike TS also fails due to steric reasons. Out-of-plane rotation of the ester produced **TS2-pyranose** and **TS3-pyranose**, which have some different structural features. In contrast to lactone **1**, the *s-trans* conformer (**TS2-pyranose**) gave the opposite stereoisomer of **TS1-pyranose**. Both **TS2-pyranose** and **TS3-pyranose** have the 6-membered TS in a twist conformation. We attribute the twist conformation to the *trans*-junction at the pyranose ring. In any case, the energy difference between the boat and twist conformations in cyclohexane is smaller (1-1.5 kcal/mol) and considerably lower than the energy associate with the barrier of rotation to a perpendicular conformation in the ester (10-13 kcal/mol). For geometries of the mimic TS structures, see Figure 2 on the next page.

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(3) HyperChem®, Version 6.0, Hypercube, Inc. MM+ supplements the Allinger's standard parameter for MM2 force field. (a) Allinger, N. A. *J. Am. Chem. Soc.*, **1997**, *99*, 8127.

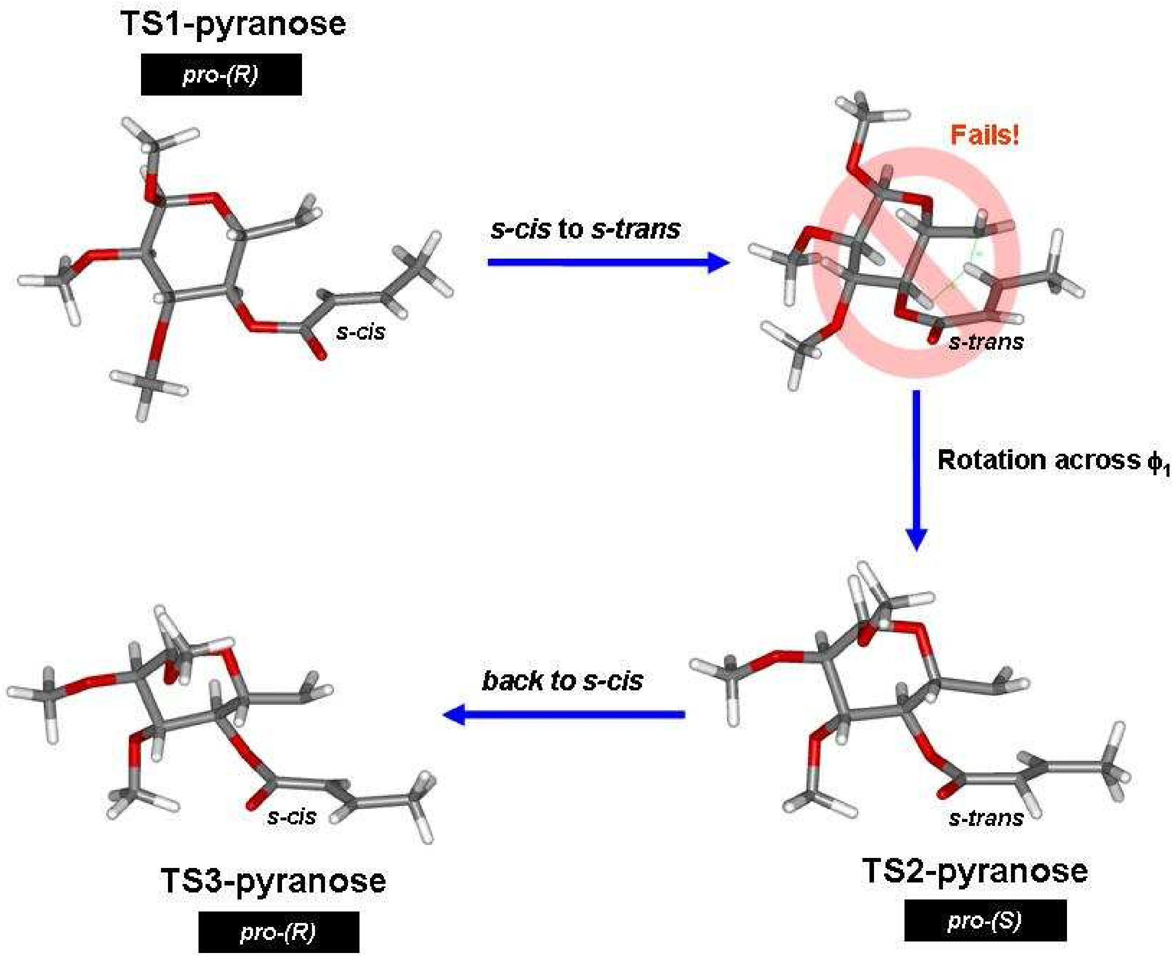


FIGURE 2. 6-*exo* transition state mimics of lactone **2**.

Table 1. Sum of electronic and thermal free energies (au/particle).

Structure	Basis Set	Electronic + Thermal Free Energies
s-cis, Z ester	3-21G(d,p)/6-31G(d,p)	-839.719348
	6-31G(d,p)	-842.010393
S trans, Z ester	3-21G(d,p)/6-31G(d,p)	-839.718228
	6-31G(d,p)	-842.009357
R1	3-21G(d,p)/6-31G(d,p)	-839.707854
	6-31G(d,p)	-841.997612
TS1	3-21G(d,p)/6-31G(d,p)	-839.696196
	6-31G(d,p)	-841.978999
	6-311G++(2d,2p)	-842.207438
TS2	3-21G(d,p)/6-31G(d,p)	-839.693694
	6-31G(d,p)	-841.976210
	6-311G++(2d,2p)	-842.204856

1 au = 627.51 $kcal.mol^{-1}$

Table 1 (continuation). Sum of electronic and thermal free energies (au/particle)**.**

Structure	Basis Set	Electronic + Thermal Free Energies
TS3	3-21G(d,p)/6-31G(d,p)	-839.695861
	6-31G(d,p)	-841.976417
	6-311G++(2d,2p)	-842.203247
TS4	3-21G(d,p)/6-31G(d,p)	-839.683176
	6-31G(d,p)	-841.966186
	6-311G++(2d,2p)	-842.195454
P1	3-21G(d,p)/6-31G(d,p)	-839.720613
	6-31G(d,p)	-842.011508
P2	3-21G(d,p)/6-31G(d,p)	-839.718872
	6-31G(d,p)	-842.010532
P3	3-21G(d,p)/6-31G(d,p)	-839.721569
	6-31G(d,p)	-842.012757
P4	3-21G(d,p)/6-31G(d,p)	-839.723960
	6-31G(d,p)	-842.018915

1 au = 627.51 kcal.mol^{-1}

Table 2. Relative Gibbs free energies (*G*, kcal.mol^{-1}), Maxwell-Boltzmann-weighted population (*P%*) and stereoselectivity for different basis sets.

Basis set		TS1	TS2	TS3	Stereoselectivity (%)
MIX[4]	*G*	0	1.6	0.2	**59**
	%P	53.9	5.5	40.6	
6-31G(d,p)	*G*	0	1.8	2.1	**96**
	%P	88.8	6.8	4.4	
6-311++G(2d,2p)	*G*	0	1.6	2.6	**98**
	%P	89.0	9.0	2.2	

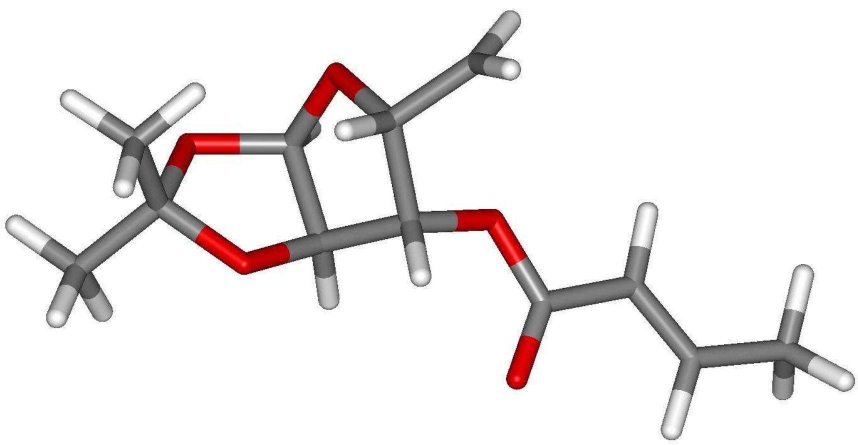
(4) While studying haloacetal radical cyclizations, Corminboeuf and co-workers observed that the most important parameter was the basis set. The energy differences were pronounced when 3-21G was used whereas 6-311G(d,p) accurately predicted the stereochemistry of the cyclizations. Corminboeuf, O.; Renaud, P.; Schiesser, C. H. *Chem. Eur. J.* **2003**, *9*, 1578.

5. Cartesian coordinates

RAD1 [*Z* ester, *s-cis*]
IFreq = 0

C	-0.372985	0.539727	0.520391
C	-0.419781	-0.250900	-0.771236
C	-1.823999	-0.895259	-0.791311
O	-2.269649	-0.892408	0.604938
C	-1.256713	-0.319400	1.460381
O	0.466488	-1.409549	-0.580221
C	-0.261061	-2.644057	-0.968168
O	-1.618618	-2.206797	-1.334749
C	-0.319729	-3.574451	0.235461
C	0.387074	-3.240482	-2.207317
C	-1.905083	0.403351	2.575468
O	-0.998309	1.821473	0.342679
C	-0.174753	2.858495	0.017651
O	1.007565	2.722618	-0.229208
C	-0.921750	4.133870	0.033007
C	-0.314144	5.285130	-0.280429
C	-0.959445	6.633722	-0.272717
H	0.736887	5.233209	-0.563851
H	-0.382744	7.335065	0.342748
H	-0.981027	7.056596	-1.285495
H	-1.984282	6.598713	0.107413
H	0.647145	0.671885	0.881061
H	-0.162494	0.321502	-1.666523
H	-2.580678	-0.407180	-1.402143
H	-0.594533	-1.109274	1.845902
H	-1.373264	0.575700	3.503799
H	-0.901335	-3.093180	1.024076
H	-0.814212	-4.509987	-0.041293
H	0.691286	-3.785414	0.594718
H	1.415754	-3.533226	-1.980513
H	-0.178663	-4.114732	-2.541128
H	0.393013	-2.493606	-3.005401
H	-1.967066	4.091812	0.325668
H	-2.860888	0.883545	2.408122

RAD1 [*Z* ester, *s-cis*]

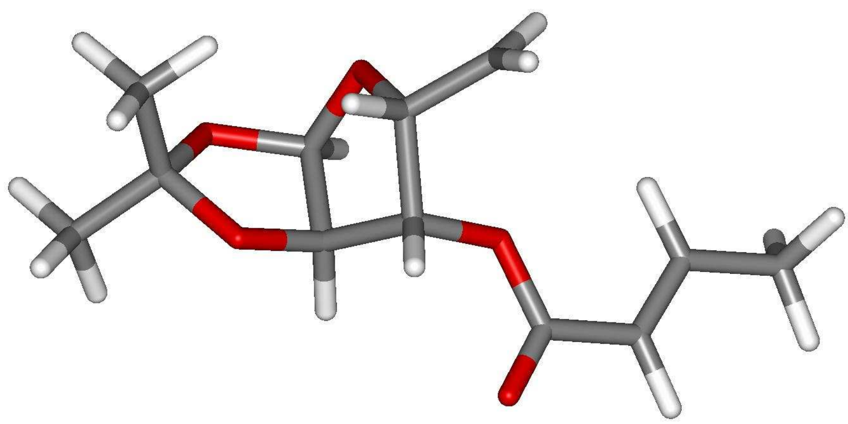


RAD2 [*Z* ester, *s-trans*]

IFreq = 0

O	-1.600998	-2.227249	-1.339277
C	-1.801667	-0.922486	-0.781148
C	-0.396735	-0.281055	-0.759527
O	0.482249	-1.444315	-0.561144
C	-0.245896	-2.672878	-0.971572
O	-2.236773	-0.936515	0.620189
C	-1.221317	-0.360524	1.468982
C	-0.362259	0.519106	0.527135
O	-1.033841	1.774656	0.333411
C	-0.254838	2.856143	0.044240
C	-1.019442	4.119918	0.013124
C	-2.304164	4.246437	0.372144
C	-3.064872	5.535615	0.376107
C	-1.863346	0.336593	2.603990
C	-0.318041	-3.620343	0.217561
C	0.406352	-3.255185	-2.215288
O	0.940997	2.782560	-0.158194
H	-2.840418	3.355992	0.695450
H	-3.971711	5.454251	-0.236088
H	-3.396662	5.781020	1.393432
H	-2.461885	6.366280	-0.001007
H	0.652386	0.685979	0.887964
H	-0.134991	0.286618	-1.656678
H	-2.561139	-0.424991	-1.380807
H	-0.540566	-1.145765	1.833785
H	-1.295316	0.579711	3.494315
H	-0.900381	-3.145525	1.009915
H	-0.820232	-4.545924	-0.078129
H	0.688951	-3.846817	0.578324
H	1.431347	-3.558179	-1.985871
H	-0.162865	-4.121912	-2.563188
H	0.422096	-2.498886	-3.004361
H	-0.430923	4.976809	-0.303172
H	-2.876262	0.701534	2.493605

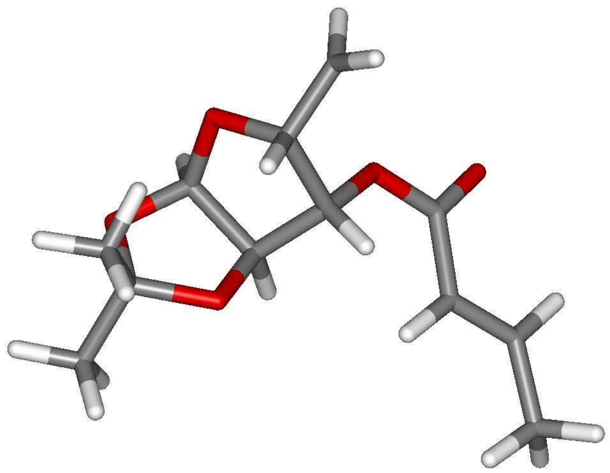
RAD2 [*Z* ester, *s-trans*]



RAD3 [*E* ester, *s-cis*]
IFreq = 0

C	1.980862	3.843360	-0.290988
C	3.435283	3.839469	-0.634963
H	1.486162	4.807911	-0.186859
H	3.613761	4.391885	-1.566302
H	4.017392	4.351634	0.142041
H	3.827862	2.825679	-0.752460
C	-0.202865	-2.617034	-0.967901
O	-1.507045	-2.106945	-1.418805
C	-1.718165	-0.818164	-0.823368
C	-0.296032	-0.238748	-0.634580
O	0.528761	-1.435979	-0.437624
O	-2.294966	-0.873008	0.519906
C	-1.349811	-0.391344	1.499092
C	-0.357998	0.493019	0.693846
O	-0.948652	1.782582	0.508275
C	-0.216685	2.902700	0.215585
C	1.228957	2.749653	-0.100346
C	-2.070706	0.287084	2.596181
C	-0.395017	-3.621402	0.159710
C	0.525207	-3.158144	-2.188452
O	-0.794717	3.966937	0.212134
H	0.609579	0.557906	1.194955
H	0.049324	0.367327	-1.478008
H	-2.390975	-0.263387	-1.473061
H	-0.748339	-1.225803	1.889734
H	-1.647148	0.323550	3.593240
H	-1.026908	-3.173092	0.928792
H	-0.895193	-4.513160	-0.228074
H	0.573634	-3.899195	0.583571
H	1.532911	-3.478142	-1.909779
H	-0.027196	-4.006397	-2.601246
H	0.590870	-2.373259	-2.946416
H	1.668822	1.762729	-0.196497
H	-2.962668	0.857879	2.372668

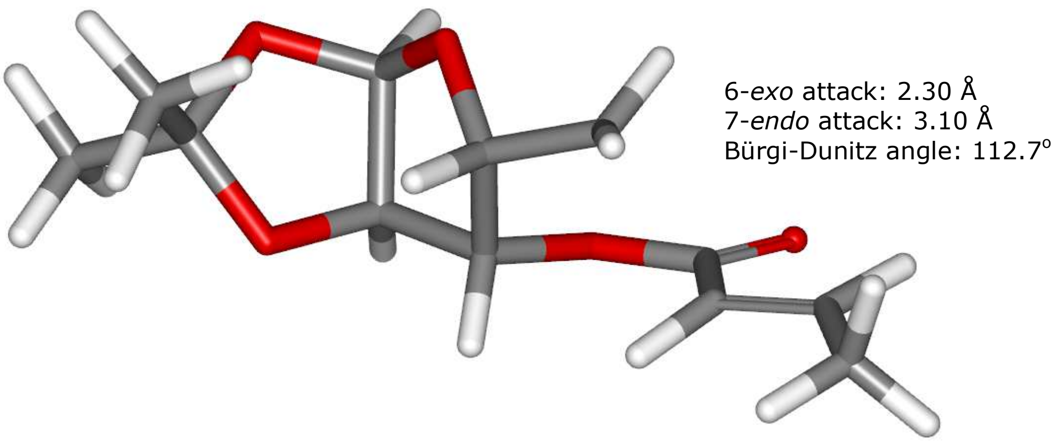
RAD3 [*E* ester, *s-cis*]



TS1 [6-*exo*, boat, *E* ester, *s-cis*, pro-(*S*)]
IFreq = 1 (-380 cm^{-1})

O	-2.268085	0.061307	-0.792754
C	-0.893245	-0.161287	-1.259310
C	-0.386673	1.275404	-1.514014
O	-1.551286	2.007040	-1.914816
C	-2.720833	1.398155	-1.258175
C	-0.099263	-0.639311	-0.065305
C	0.068755	0.665933	0.758511
O	0.168053	1.716297	-0.226045
C	1.270959	0.694046	1.640775
O	1.140242	-1.117545	-0.587443
C	2.173601	-1.463800	0.243926
O	3.250573	-1.699345	-0.253262
C	-3.126753	2.218970	-0.042540
C	-3.806740	1.229390	-2.309262
C	1.893064	-1.516706	1.705662
C	2.928663	-1.750410	2.572356
C	2.771170	-1.981511	4.039184
H	-0.628149	-1.420614	0.488595
H	-0.842918	-0.818151	-2.131440
H	0.366053	1.404048	-2.288088
H	-0.851691	0.782075	1.347823
H	2.164976	1.134946	1.213167
H	1.137044	0.816593	2.709537
H	-2.239888	2.406265	0.566249
H	-3.542083	3.179041	-0.362282
H	-3.873049	1.673670	0.541863
H	-4.676423	0.737884	-1.865034
H	-4.097907	2.207775	-2.701349
H	-3.423655	0.616962	-3.129834
H	0.878708	-1.719038	2.037804
H	3.937875	-1.701391	2.170332
H	3.350237	-2.855572	4.363118
H	3.159550	-1.129398	4.616113
H	1.726817	-2.134424	4.329138

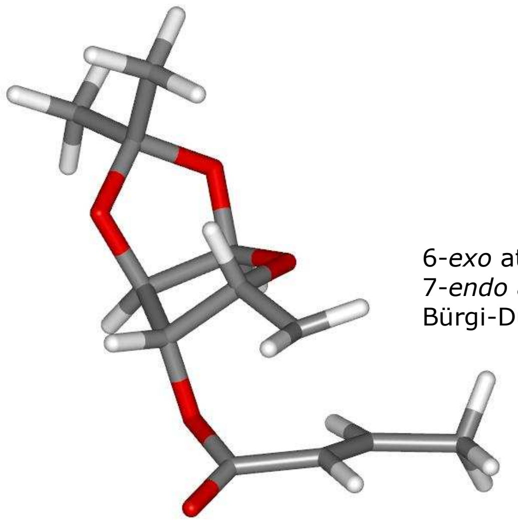
TS1 [6-*exo*, boat, *E* ester, *s-cis*, pro-(*S*)]



TS2 [6-*exo*, chair, *E* ester, *s-trans*, pro-(*S*)]
IFreq = 1 (-383 cm^{-1})

C	-0.501995	-1.069179	0.018013
C	0.866716	-1.068092	-0.630463
C	1.421427	0.357107	-0.352852
O	0.262451	1.159900	0.046576
C	-0.937380	0.401693	-0.178723
O	0.653965	-1.070535	-2.081323
C	1.534022	-0.056912	-2.693269
O	2.030021	0.778535	-1.581375
C	0.699780	0.786076	-3.646348
C	2.739657	-0.727979	-3.337666
C	-2.016510	0.902455	0.714154
O	-0.286292	-1.374053	1.400295
C	-1.402145	-1.132594	2.201808
O	-2.274816	-1.956500	2.331761
C	-1.387020	0.212633	2.809903
C	-0.225933	0.869795	3.136983
C	-0.176199	2.145309	3.912377
H	-1.191525	-1.788672	-0.435355
H	1.518939	-1.878722	-0.294661
H	2.163825	0.439278	0.437618
H	-1.251188	0.481204	-1.237007
H	-1.999473	1.967946	0.918041
H	-3.001330	0.454923	0.603936
H	-0.088955	1.293236	-3.085213
H	1.332853	1.537713	-4.125176
H	0.249280	0.145043	-4.408937
H	2.409667	-1.395192	-4.138381
H	3.408708	0.032749	-3.748042
H	3.281877	-1.309185	-2.586468
H	-2.319531	0.495331	3.290744
H	0.708916	0.480178	2.749127
H	0.531374	2.076072	4.748285
H	0.176569	2.969667	3.275758
H	-1.154878	2.422813	4.314436

TS2 [6-*exo*, chair, *E* ester, *s-trans*, pro-(*S*)]

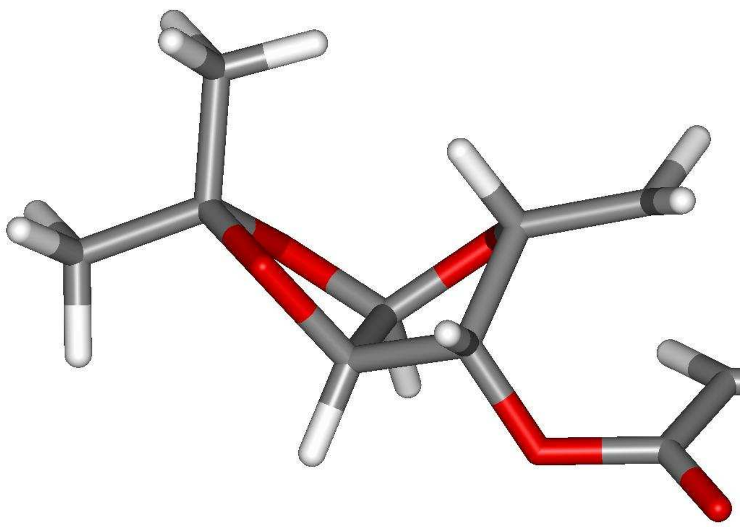


6-*exo* attack: 2.29 Å
7-*endo* attack: 3.01 Å
Bürgi-Dunitz angle: 107.8°

TS3 [6-*exo*, chair, *E* ester, *s*-*cis*, pro-(*R*)]
IFreq = 1 (-359 cm^{-1})

C	-0.384439	-1.109727	-0.070196
C	1.027758	-1.081605	-0.626152
C	1.497622	0.379449	-0.402561
O	0.259488	1.154357	-0.196231
C	-0.875295	0.295799	-0.449086
O	0.911779	-1.166406	-2.088128
C	1.796121	-0.149956	-2.694592
O	2.216925	0.733335	-1.587673
C	0.990531	0.644717	-3.712204
C	3.043936	-0.815713	-3.256614
C	-2.062046	0.793511	0.289006
O	-0.252910	-1.348859	1.334756
C	-1.189869	-0.881974	2.250062
O	-1.839932	-1.671259	2.892939
C	-1.208240	0.592154	2.420778
C	-1.993964	1.152881	3.390265
C	-1.983602	2.602800	3.751003
H	-0.997429	-1.898614	-0.520237
H	1.691357	-1.843536	-0.209786
H	2.143774	0.559390	0.452332
H	-1.070938	0.247883	-1.534392
H	-2.222718	1.865663	0.299510
H	-2.954097	0.173464	0.284735
H	0.181129	1.169497	-3.199270
H	1.635736	1.381727	-4.197930
H	0.573088	-0.030780	-4.463495
H	2.762935	-1.515177	-4.048907
H	3.719465	-0.056603	-3.660351
H	3.557788	-1.362154	-2.460867
H	-0.398225	1.149666	1.960601
H	-2.704269	0.506311	3.901993
H	-2.951006	3.073226	3.521580
H	-1.824456	2.742237	4.827885
H	-1.206395	3.154696	3.213527

TS3 [6-*exo*, chair, *E* ester, *s*-*cis*, pro-(*R*)]

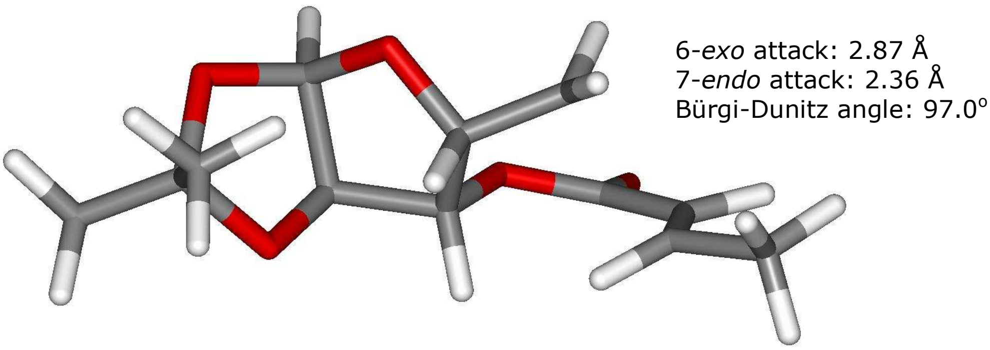


6-*exo* attack: 2.31 Å
7-*endo* attack: 3.12 Å
Bürgi-Dunitz angle: 114.0°

TS4 [7-*endo*, *E* ester, *s-trans*, pro-(S)]
IFreq = 1 (-378 cm^{-1})

O	0.569432	-3.319898	1.076651
C	-0.319824	-2.220750	0.853937
C	0.321430	-1.421125	-0.298844
O	1.757443	-1.640138	-0.075515
C	1.931891	-2.878680	0.726981
O	-0.370868	-1.279194	1.982426
C	0.113084	0.024103	1.580281
C	0.032659	0.031002	0.028269
O	-1.269571	0.273305	-0.511495
C	-1.851965	1.505324	-0.720734
C	-1.464550	2.684449	0.069842
C	-0.360492	2.898323	0.849321
C	-0.195281	4.162683	1.650094
C	-0.674403	1.064184	2.305123
C	2.705631	-2.526111	1.989081
C	2.560933	-3.961732	-0.134624
O	-2.783976	1.544413	-1.495878
H	0.778872	0.682936	-0.431937
H	-0.006730	-1.728579	-1.294580
H	-1.312624	-2.629776	0.680561
H	1.180864	0.115913	1.824666
H	-1.752865	0.948717	2.287163
H	-0.256501	1.495814	3.209587
H	2.097207	-1.846929	2.589405
H	2.898823	-3.431093	2.572465
H	3.653932	-2.050056	1.725240
H	3.571593	-3.664027	-0.426964
H	2.603239	-4.900243	0.424621
H	1.953932	-4.108270	-1.031223
H	-2.267456	3.417157	0.093965
H	0.560694	2.356062	0.675844
H	0.436435	4.875749	1.104857
H	-1.155843	4.644364	1.851775
H	0.300160	3.964028	2.605104

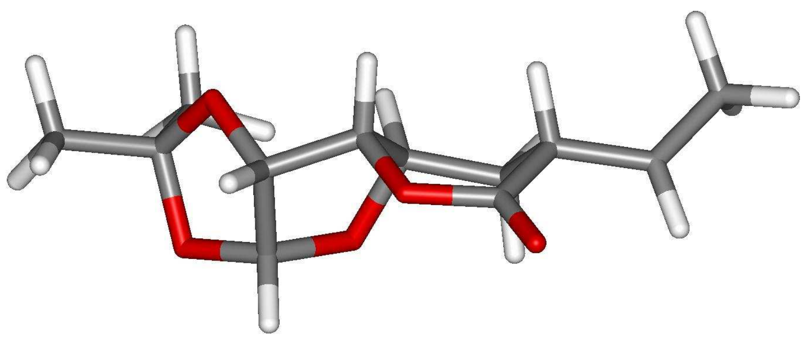
TS4 [7-*endo*, *E* ester, *s-trans*, pro-(*S*)]



P1 [6-*exo*, boat, (*S*)]
IFreq = 0

O	0.004178	1.854506	0.008516
C	-0.395278	1.476579	-1.358186
C	-0.809643	-0.006928	-1.254361
C	-0.088072	-0.515283	-0.024548
C	-0.073397	0.719750	0.889893
O	-1.567754	2.154141	-1.814431
C	-2.740605	1.424125	-1.300553
O	-2.234764	0.083137	-0.906003
C	-3.287860	2.118882	-0.060900
C	-3.729870	1.282229	-2.445349
O	1.231648	-0.884265	-0.456538
C	2.224169	-1.023421	0.476807
C	1.826819	-0.656880	1.903827
C	2.981337	-0.718163	2.847240
C	2.781365	-0.925210	4.310033
C	1.125442	0.737419	1.844928
O	3.319594	-1.371504	0.115245
H	-0.597031	-1.374540	0.423871
H	-0.630873	-0.594834	-2.158471
H	0.416583	1.716222	-2.041320
H	-1.023902	0.733830	1.437685
H	1.825748	1.483808	1.460204
H	0.833422	1.043487	2.853113
H	-2.461043	2.310031	0.625534
H	-3.739322	3.075322	-0.340128
H	-4.040180	1.486246	0.417478
H	-4.609888	0.726995	-2.109336
H	-4.032606	2.273531	-2.793472
H	-3.255707	0.745233	-3.270715
H	1.063018	-1.384413	2.227050
H	3.964399	-0.469240	2.460983
H	3.674832	-1.353480	4.778666
H	2.570091	0.013538	4.852391
H	1.937744	-1.597724	4.515923

P1 [6-*exo*, boat, (*S*)]

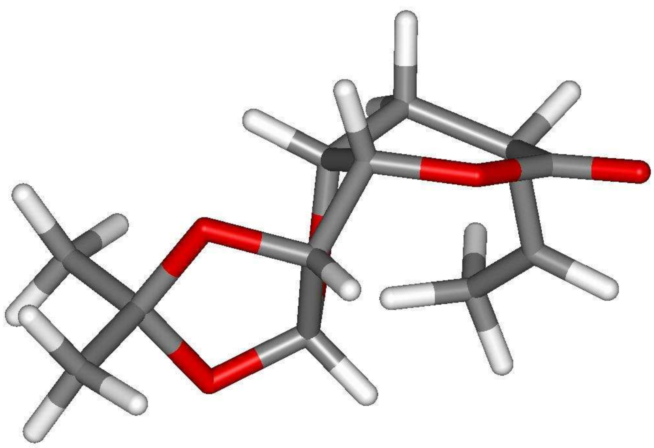


P2 [6-*exo*, half-chair, (*S*)]

IFreq = 0

O	2.060998	0.651921	-1.172066
C	1.221029	0.180806	-0.118805
C	0.696705	-1.191016	-0.601088
O	0.670392	-1.030606	-2.062068
C	1.567530	0.087666	-2.444004
O	0.006624	0.996579	0.073399
C	-1.169545	0.230362	-0.242556
C	-0.748698	-1.236322	-0.141843
O	-0.761804	-1.791495	1.185409
C	-1.377413	-1.234431	2.270760
C	-1.958124	0.178468	2.161600
C	-1.024778	1.100129	2.914316
C	-0.843979	2.543558	2.588031
C	-2.292398	0.577910	0.714315
C	0.755953	1.134604	-3.194437
C	2.769744	-0.454091	-3.200904
O	-1.387101	-1.862598	3.300403
H	-1.353650	-1.886827	-0.779250
H	1.302601	-2.042015	-0.280164
H	1.797490	0.195334	0.802836
H	-1.468513	0.414886	-1.282402
H	-2.526121	1.644245	0.651250
H	-3.191581	0.040662	0.386237
H	0.003429	1.546292	-2.519614
H	1.414146	1.945138	-3.520065
H	0.273390	0.681480	-4.064400
H	2.439813	-0.929896	-4.128165
H	3.457409	0.363630	-3.432245
H	3.285363	-1.190526	-2.579520
H	-2.904351	0.117803	2.726426
H	-0.673045	0.714921	3.867480
H	-0.138952	3.011395	3.281279
H	-0.457584	2.655983	1.568963
H	-1.785195	3.117129	2.650415

P2 [6-*exo*, half-chair, (*S*)]

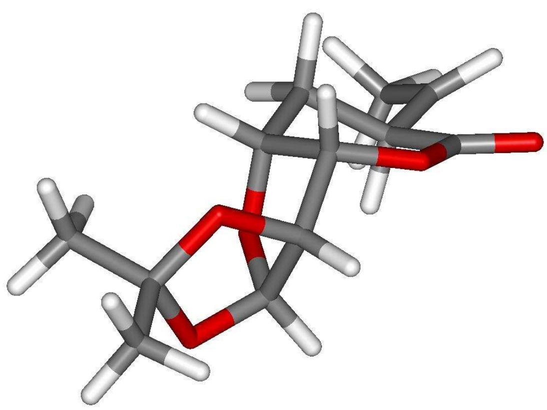


P3 [6-*exo*, half-chair, (*R*)]

IFreq = 0

C	0.191259	-2.817970	3.839333
C	0.684004	-2.056918	2.625838
C	1.743047	-1.010907	2.980717
O	1.536235	-0.333519	4.232906
C	0.691715	-0.754409	5.227696
C	-0.350910	-1.812520	4.883635
C	1.572534	0.006849	1.869748
C	0.060431	-0.022001	1.540572
O	-0.417029	-1.312551	2.069024
O	2.171338	-0.592176	0.667927
C	1.229789	-0.443145	-0.464661
O	-0.019341	0.086126	0.118403
C	0.980429	-1.818578	-1.066790
C	1.755315	0.596600	-1.443032
O	0.780409	-0.215924	6.302986
C	-0.924899	-2.443403	6.110805
C	-2.149088	-3.292707	6.042114
H	2.752281	-1.431567	2.994171
H	1.970444	1.000359	2.090786
H	-0.553014	0.768785	1.966475
H	1.115869	-2.728811	1.873410
H	-0.603737	-3.510765	3.547315
H	1.008965	-3.415545	4.260871
H	0.476602	-2.444509	-0.326773
H	0.338822	-1.726543	-1.947268
H	1.932413	-2.274232	-1.352000
H	2.702622	0.257847	-1.870860
H	1.026447	0.750047	-2.243756
H	1.912458	1.543348	-0.919762
H	-1.138497	-1.263599	4.339168
H	-0.396297	-2.315469	7.049476
H	-1.950070	-4.304847	5.648266
H	-2.595126	-3.426330	7.032830
H	-2.913040	-2.854778	5.383993

P3 [6-*exo*, half-chair, (*R*)]



P4 [7-*endo*, twist-boat, (*S*)]

IFreq = 0

C	-0.010195	0.015047	0.049316
C	0.018249	0.047430	1.562540
C	1.518962	0.000193	1.921293
O	2.164544	-0.622530	0.752277
C	1.189347	-0.886366	-0.273201
O	-0.460041	-1.264001	2.026096
C	0.491893	-1.789532	3.039380
O	1.584900	-0.803202	3.104573
C	1.029870	-3.128402	2.553072
C	-0.181124	-1.822414	4.400916
C	1.821652	-0.610504	-1.630103
C	0.803219	-0.521380	-2.781318
C	-0.025220	-1.819946	-2.960157
O	0.179770	1.370121	-0.381247
C	-0.135432	1.707853	-1.675318
O	-0.413139	2.870055	-1.920539
C	-0.080083	0.693941	-2.716750
H	-0.955938	-0.382893	-0.329388
H	-0.532039	0.880362	2.006438
H	2.005712	0.948582	2.133048
H	0.850271	-1.927324	-0.195662
H	2.382247	0.326215	-1.550820
H	2.554054	-1.394850	-1.848629
H	1.623335	-2.956244	1.653787
H	1.674766	-3.568373	3.319428
H	0.200729	-3.807433	2.336690
H	-0.995123	-2.553367	4.397932
H	0.550303	-2.094306	5.167009
H	-0.586423	-0.833179	4.627113
H	-0.621642	0.973316	-3.616627
H	1.384837	-0.407213	-3.711727
H	0.643748	-2.669594	-3.129123
H	-0.634415	-2.038378	-2.078063
H	-0.700848	-1.739737	-3.817017

P4 [7-*endo*, twist-boat, (*R*)]