

A Combined Computational and Experimental Investigation of the Oxidative Ring-Opening of Cyclic Ethers by Oxoammonium Cations

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General Considerations:

General:

Quantum chemical calculations were performed using Gaussian 09.¹ All optimized geometries were calculated using B3LYP², a hybrid density functional, with the 6-31G(d) basis set³. Stationary points were characterized by frequency calculations at 298 K, with structures at energy minima showing no negative frequencies and transition-states showing one negative frequency. The Gibbs free energies were calculated by the sum of electronic and thermal free energy. The thermal free energy thermodynamic correction factor was obtained via frequency analysis. All energetic values shown are in kcal mol⁻¹ and molecular structures were generated using CYLView.⁴

¹ Frisch, M. J. et al. Gaussian 09, revision B.02; Gaussian, Inc.: Wallingford, CT, **2009**

² (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648; (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785; (c) Vosko, S. H.; Wilk, L.; Nusair, M. *Can. J. Phys.* **1980**, *58*, 1200; (d) Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623.

³ (a) Ditchfield, R.; Hehre, W. J.; Pople, J. A. *J. Chem. Phys.*, **1971**, *54*, 724; (b) Hehre, W. J.; Ditchfield, R.; Pople, J. A. *J. Chem. Phys.*, **1972**, *56*, 2257; (c) Hariharan, P. C.; Pople, J. A. *Theor. Chim. Acta*, **1973**, *28*, 213.

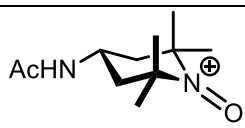
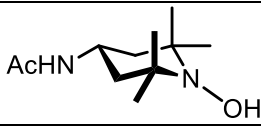
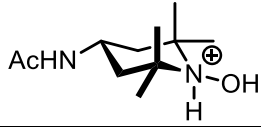
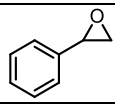
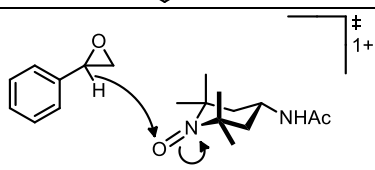
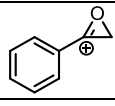
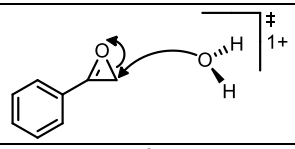
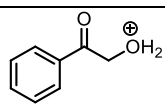
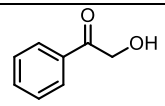
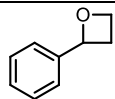
⁴ Legault, C. Y. CYLview, 1.0b. Université de Sherbrooke; **2009**. <http://www.cylview.org>.

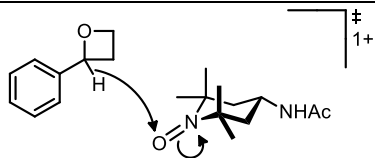
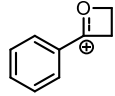
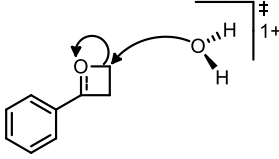
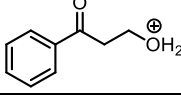
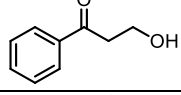
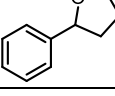
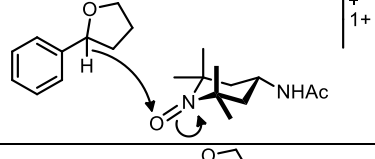
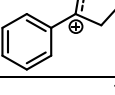
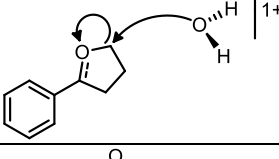
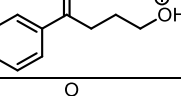
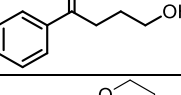
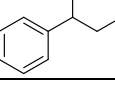
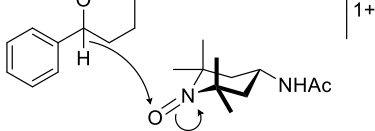
Complete Citation for Gaussian 09:

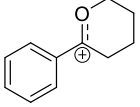
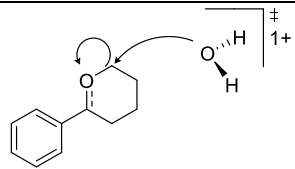
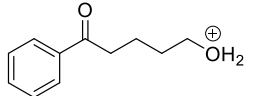
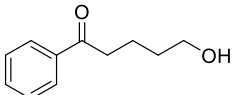
Gaussian 09, Revision **A.02**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2009**.

Summary of Energies

Table S1. Summary of SCF energy and thermal correction factor for Gibbs free energy, obtained from the optimization and frequency calculations, respectively.

identifier	system	thermal correction for Gibbs Free Energy ^a	SCF energy ^a
1		0.2744	-691.480091
		0.28433	-692.332833
		0.30036	-692.710764
	H ₂ O	0.0035	-76.4089533
		0.10709	-384.846008
		0.39577	-1076.29824
		0.09611	-383.966128
		0.11665	-460.388439
		0.12194	-460.452794
		0.10863	-460.093655
2a		0.13469	-424.162711

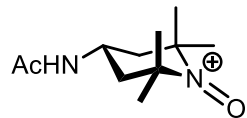
		0.42588	-1115.64054
		0.1249	-423.32048
		0.14522	-499.720222
		0.15019	-499.780175
3a		0.13691	-499.419341
2e		0.16253	-463.504432
		0.45498	-1154.98738
		0.15368	-462.672665
		0.17538	-539.049878
		0.17593	-539.101813
3e		0.16150	-538.727428
2j		0.19200	-502.824113
		0.48183	-1194.29427

		0.18125	-501.986555
		0.20111	-578.368670
		0.20442	-578.417000
3j		0.18773	-578.038582

^aEnergetic values in Hartrees

Cartesian Coordinates of Stationary Points

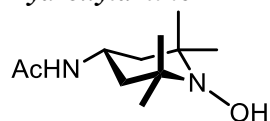
1 Oxoammonium Cation



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	0.19337000	1.19677000	-0.56031100
C	-1.24311100	1.37185800	-0.02128600
C	-1.35064000	-1.34694900	0.04200200
C	0.09046200	-1.31164300	-0.51157400
C	0.90218700	-0.08142100	-0.08907100
H	0.16395400	1.21135800	-1.65658900
H	0.75791200	2.07833800	-0.24071600
H	0.58152200	-2.22555600	-0.16328800
H	0.04736200	-1.36538000	-1.60649200
H	1.03616600	-0.06349800	0.99501700
N	-1.99263600	0.03617500	-0.16654000
O	-3.15470200	0.07579300	-0.44104900
C	-1.39380700	-1.62971400	1.56785800
H	-2.40543400	-1.51093800	1.96488800
H	-1.09659200	-2.67556800	1.69018800
H	-0.70290100	-1.01406000	2.14276900
C	-2.20973300	-2.37232800	-0.70320600
H	-2.32326900	-2.10920200	-1.75895500
H	-1.69250800	-3.33415200	-0.64235600
H	-3.19817300	-2.48552700	-0.25324600
C	-1.27293300	1.72904500	1.48938600
H	-0.91905600	2.76156000	1.56440600
H	-2.29077500	1.68497900	1.88544000
H	-0.61828800	1.10369100	2.09556200
C	-2.01660800	2.42497700	-0.82019200
H	-1.42244700	3.34301000	-0.80538000
H	-2.15191100	2.11991900	-1.86202500
H	-2.99212300	2.64099200	-0.37949100
N	2.24918600	-0.15330200	-0.63514000
H	2.35492200	-0.27807200	-1.63473900
C	3.37429200	-0.00933200	0.12427100
C	4.69153600	-0.09459800	-0.61965500
H	4.57646900	-0.26406500	-1.69382900
H	5.24576400	0.83665200	-0.46391500
H	5.28578000	-0.90896400	-0.19271200
O	3.32691400	0.17600400	1.34578600

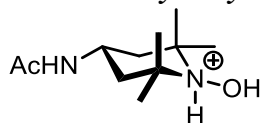
Hydroxylamine



Coordinates (from last standard orientation):

ATOM	X	Y	Z
0 1			
C	0.03893700	0.00893900	-0.00136400
C	0.01443400	0.04178300	1.54643000
C	2.58770900	0.00690300	1.54834100
C	2.56748100	-0.02390500	-0.00017500
C	1.31305500	0.63260900	-0.59735400
H	-0.02849500	-1.03539500	-0.33287000
H	-0.84396900	0.52998700	-0.39205100
H	3.46535000	0.47436000	-0.38657500
H	2.61133600	-1.07067300	-0.32939800
H	1.32512900	1.70858500	-0.40860300
C	3.73358600	-0.88404500	2.06781400
H	4.69201700	-0.47616400	1.72783800
H	3.74021400	-0.89660000	3.16476600
H	3.65062600	-1.91090000	1.70760700
C	2.87285700	1.43045400	2.07938200
H	2.67666900	1.48639300	3.15528500
H	3.93162000	1.65910200	1.91584700
H	2.30117500	2.21553000	1.58471900
C	-0.23295900	1.47257500	2.07675000
H	-1.28458100	1.73014400	1.91010500
H	-0.03842200	1.52318000	3.15326000
H	0.36085900	2.24214100	1.58366700
C	-1.15545900	-0.81823500	2.06425600
H	-1.16443300	-0.83107800	3.16125200
H	-2.10208100	-0.38488100	1.72277500
H	-1.09949000	-1.84680000	1.70360400
N	1.29362900	-0.51551400	2.12594800
O	1.27475700	-1.93994000	1.78934400
H	1.26562900	-2.36681200	2.66044600
N	1.32173200	0.50205700	-2.05578300
H	1.44751400	-0.42753400	-2.43809700
C	1.10699000	1.52303000	-2.92344600
C	1.12922600	1.16069400	-4.39780300
H	1.88224500	1.77490800	-4.90223100
H	1.34815900	0.10553400	-4.58607100
H	0.15590200	1.40413800	-4.83690100
O	0.90622100	2.69057500	-2.55465100

Protonated hydroxylamine



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-0.12312700	-0.12449600	0.06497400
C	-0.04723800	-0.07035800	1.59993800
C	2.65490700	0.05976000	1.29867600
C	2.38752800	0.00319600	-0.21113100
C	1.03112900	0.60220100	-0.63454000
H	-0.14999100	-1.17456500	-0.25211200
H	-1.07948900	0.32348800	-0.22679800
H	3.18464900	0.56081400	-0.71170900
H	2.44327700	-1.03668000	-0.55400800
H	1.02461100	1.66452100	-0.37439700
C	3.86673500	-0.80705200	1.68505700
H	4.76524500	-0.32435600	1.29194800
H	4.00156500	-0.88043900	2.77266700
H	3.84445800	-1.80655500	1.23915300
C	2.89078100	1.48039200	1.83783700
H	2.88234600	1.51199000	2.93409400
H	3.88754800	1.79497900	1.51705800
H	2.19222600	2.22234200	1.45755100
C	-0.27876200	1.33830800	2.17170100
H	-1.34961000	1.54700700	2.09900400
H	-0.01696200	1.40078200	3.23437200
H	0.23810400	2.13091000	1.63465000
C	-1.05564400	-1.03021400	2.25067700
H	-0.95200000	-1.04793000	3.34173500
H	-2.05888400	-0.65781500	2.02419400
H	-0.97511500	-2.04837400	1.87196900
N	1.39494100	-0.55759400	2.01875900
O	1.36686800	-1.96717800	1.84912400
H	2.22543300	-2.29232100	2.18016100
H	1.47894400	-0.37387400	3.02792500
N	0.86386000	0.56406400	-2.07587900
C	1.49870700	1.50457300	-2.85980100
C	1.28270700	1.38703300	-4.35438200
H	0.84132000	2.31989800	-4.71802700
H	2.25364300	1.27566500	-4.84645000
H	0.63664300	0.55264400	-4.64261500
O	2.18412200	2.38144100	-2.34840500
H	0.38826400	-0.21714800	-2.50619000

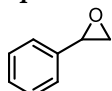
Water

H₂O

Coordinates (from last standard orientation):

ATOM	X	Y	Z
0 1			
O	0.00000000	0.00000000	0.11972000
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H	0.00000000	-0.76156000	-0.47887900

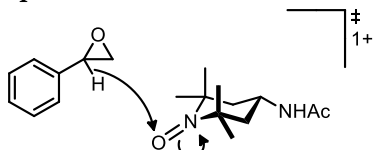
Epoxide SM



Coordinates (from last standard orientation):

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C	-5.66587200	2.41727600	1.12233100
C	-4.55614000	2.64491700	1.93809400
C	-3.54403300	3.50754400	1.51634300
C	-3.62604800	4.14350100	0.27182500
C	-4.74573200	3.91847800	-0.53875000
C	-5.75874300	3.05938500	-0.11495200
H	-6.45727800	1.74942200	1.45185700
H	-4.48049900	2.15602200	2.90580100
H	-2.68370400	3.68856500	2.15741500
H	-4.81992000	4.44001200	-1.48827000
H	-6.62630700	2.89549100	-0.74889000
C	-2.51913900	5.03730300	-0.17840800
C	-1.84408800	4.86404200	-1.48157800
O	-2.78285700	5.92238600	-1.27681200
H	-1.93485700	5.49081400	0.62493100
H	-2.17648600	4.06478600	-2.14429800
H	-0.80531900	5.17455400	-1.60169500

Epoxide TS1

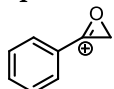


Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-5.82484200	5.24488300	-0.61761800
C	-5.60094900	4.56588500	0.58850900
C	-4.30943800	4.22250500	0.95995100
C	-3.22960700	4.54523100	0.10287000
C	-3.45915800	5.24239700	-1.10742700
C	-4.75706800	5.58023700	-1.46192500
H	-6.83809200	5.51220700	-0.90226300

H	-6.43716500	4.30597500	1.22948600
H	-4.12155100	3.69446500	1.89037400
H	-2.62377600	5.47823200	-1.75917800
H	-4.94587900	6.09820200	-2.39673100
C	-1.89959400	4.17178800	0.46999900
H	-1.48115700	5.25069100	1.56674800
C	-1.03908700	3.07390200	0.87046300
O	-0.81307200	4.00799000	-0.28650600
C	-1.77193000	7.57254000	3.24660500
C	0.31614200	7.48855000	1.58963000
C	0.71844400	8.86884200	2.15675600
C	-0.47651700	9.70828200	2.60655000
C	-1.23697400	8.94768100	3.70192300
H	1.39142200	8.71220800	3.01133000
H	1.29163500	9.39539700	1.38619900
H	-1.15186700	9.89856900	1.76738100
H	-0.56950600	8.80500700	4.56173000
H	-2.08633300	9.54853200	4.03962000
N	-0.67701500	6.86518200	2.51626000
O	-0.83156000	5.55405500	2.38733300
C	-2.14275300	6.73500900	4.48358900
H	-2.84894900	7.30419900	5.09553600
H	-2.61451300	5.78773600	4.21096300
H	-1.25740000	6.51950100	5.08904100
C	-3.02194400	7.73614500	2.34615300
H	-3.36863000	6.76829700	1.97077600
H	-3.83010100	8.16721200	2.94511900
H	-2.85051100	8.40274000	1.49842500
C	1.55878100	6.58223400	1.52923600
H	1.34799900	5.63330200	1.03100700
H	2.34182900	7.09419400	0.96170100
H	1.94013000	6.37468100	2.53344400
C	-0.27922700	7.62912900	0.16626400
H	0.50021500	8.00451200	-0.50442900
H	-0.59932000	6.65825100	-0.22299900
H	-1.12119000	8.32337300	0.12549300
N	-0.05241900	11.02576000	3.05147400
C	-0.92151700	12.09107100	2.99210300
C	-0.39427700	13.40967100	3.52583100
H	-0.41965900	14.14949000	2.71990800
H	-1.06390300	13.76660700	4.31408500
H	0.62441900	13.35120700	3.92083400
O	-2.04467100	11.96939100	2.51819500
H	0.82200600	11.12161100	3.54949400
H	-0.33168300	3.21177600	1.68186100
H	-1.27538500	2.05923100	0.56091000

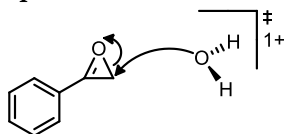
Epoxide Cation



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-5.61658300	2.47636000	1.09527200
C	-4.40468500	2.54895000	1.80157300
C	-3.41419400	3.41313600	1.37128400
C	-3.64824000	4.21180200	0.21729400
C	-4.87986200	4.13306100	-0.49427000
C	-5.85501800	3.26261600	-0.04600300
H	-6.38982600	1.79531100	1.43937700
H	-4.24855200	1.93033800	2.67878800
H	-2.46866700	3.48815000	1.89974300
H	-5.03740600	4.75176900	-1.37243400
H	-6.80117700	3.18452600	-0.57087200
C	-2.65241500	5.08166000	-0.21698600
C	-1.36222700	5.71618200	-0.16310700
O	-2.50186900	5.92600800	-1.17594200
H	-1.20634200	6.57902600	0.47845600
H	-0.49631000	5.22691300	-0.60038900

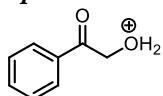
Epoxide TS2



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-5.61688100	2.48720300	1.13386600
C	-4.36440500	2.57569200	1.75478400
C	-3.40395000	3.44458200	1.25552100
C	-3.70673600	4.23082100	0.12152100
C	-4.97406400	4.13821200	-0.50224400
C	-5.92205500	3.26592400	0.00851600
H	-6.36317900	1.80496300	1.53042900
H	-4.14579600	1.96556800	2.62508700
H	-2.43120000	3.52214300	1.72801600
H	-5.18744300	4.75101000	-1.37256000
H	-6.89696800	3.18589700	-0.46101800
C	-2.75772700	5.13991500	-0.43642400
C	-1.37816100	5.59246900	-0.19025600
O	-2.83954100	5.90288900	-1.41398600
H	-1.26507000	6.59036900	0.21636400
H	-0.62627800	5.24369100	-0.88806800
O	-0.43423600	4.75566300	1.37615900
H	-0.16087800	5.39783600	2.05735900
H	0.37019300	4.26236100	1.12974400

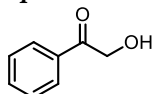
Epoxide + H2O Cation



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-3.22934900	-1.77944800	-0.72712500
C	-1.88063300	-1.58980300	-0.47791700
C	-1.43841100	-0.38730300	0.13337600
C	-2.38141900	0.61495100	0.48662100
C	-3.72675700	0.41114500	0.23133400
C	-4.14961500	-0.78167200	-0.37320500
H	-3.57323900	-2.69680300	-1.19297500
H	-1.17362500	-2.36676100	-0.75173300
H	-2.03989900	1.53186500	0.95437300
H	-4.45201100	1.17225100	0.49920200
H	-5.20653800	-0.93644200	-0.56991900
C	-0.05625400	-0.17955600	0.39010500
C	1.05981600	-1.16186800	0.06807200
H	0.84862500	-2.12597500	0.54838500
O	0.33949800	0.91462600	0.94644300
H	1.09814500	-1.32082700	-1.01701600
O	2.24765400	-0.59345600	0.58712700
H	2.97747700	-0.66165000	-0.04806400
H	1.33396300	0.84708800	1.04218800

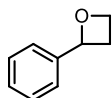
Epoxide Product



Coordinates (from last standard orientation):

ATOM	X	Y	Z
0 1			
C	-3.96527100	0.89884600	-0.39990500
C	-2.86947600	1.24925600	0.39062800
C	-2.32726100	2.53173300	0.31034600
C	-2.87771400	3.47520800	-0.57205400
C	-3.98016400	3.11221900	-1.36457900
C	-4.52204900	1.83466400	-1.27761900
H	-4.38693600	-0.10072700	-0.33201400
H	-2.43831200	0.52396500	1.07537000
H	-1.49467900	2.80976300	0.94545800
H	-4.38981600	3.85200300	-2.04450600
H	-5.37566400	1.56382100	-1.89312000
C	-2.32490800	4.85165500	-0.74942400
C	-1.12279600	5.32442200	0.07622200
O	-2.76918700	5.60890600	-1.59989300
H	-1.01813800	6.39716300	-0.12660600
H	-0.22468100	4.81307100	-0.31352200
O	-1.31440200	5.05552900	1.46104600
H	-0.56512000	5.44162900	1.93983200

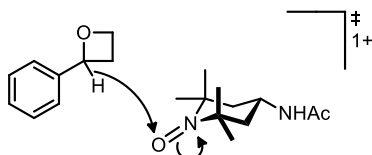
2a Oxetane SM



Coordinates (from last standard orientation):

ATOM	X	Y	Z
0 1			
C	-0.09979000	0.11110400	-0.05635500
C	-1.23199100	-0.71102300	-0.08167700
C	-0.26184100	1.48671700	0.15143100
C	-2.50326500	-0.16676500	0.10478200
H	-1.10413300	-1.77227400	-0.27007400
C	-1.53123000	2.03003700	0.34902900
H	0.61124100	2.13667400	0.15619900
C	-2.65664600	1.20337400	0.32577900
H	-3.37636000	-0.81369300	0.07420800
H	-1.64279700	3.09915700	0.51045500
H	-3.64721000	1.62626900	0.47121200
C	1.28120000	-0.47035000	-0.20970300
C	1.97565900	-1.08092600	1.04071100
H	1.93080300	0.24814900	-0.73174900
C	2.14344500	-2.32786500	0.15624900
H	1.29556100	-1.21819200	1.88477300
H	2.88837500	-0.58525800	1.38082700
H	1.73213700	-3.27043000	0.53627900
H	3.16760900	-2.50240500	-0.20047900
O	1.30986800	-1.75699700	-0.88049100

Oxetane TSI

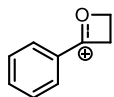


Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-6.02267200	4.99109300	-0.03341700
C	-5.56217200	4.32293900	1.10839300
C	-4.20530500	4.07000000	1.26426700
C	-3.29566100	4.47685700	0.26382500
C	-3.76387600	5.15794000	-0.87983900
C	-5.12416800	5.40578200	-1.02356600
H	-7.08444300	5.18468400	-0.15291200
H	-6.26489400	3.99693800	1.86874500
H	-3.84442000	3.54751600	2.14632400
H	-3.06153800	5.45771300	-1.65076800
H	-5.48940400	5.91458500	-1.91015700
C	-1.87861400	4.19448500	0.42659000
C	-1.16572200	2.97567400	1.00661500
H	-1.48607200	5.17343800	1.38405200
C	-0.18038400	3.22429800	-0.15367000
H	-1.74648900	2.05208400	0.93951500

H	-0.75944000	3.08741100	2.01469000
H	0.82290200	3.56535900	0.10678900
O	-1.01010500	4.34983500	-0.62418600
C	-1.93888400	7.67078200	2.94535000
C	0.41043600	7.46499600	1.68822500
C	0.78488500	8.81557500	2.34382300
C	-0.41598900	9.72262800	2.60544500
C	-1.40182400	8.99499300	3.53058200
H	1.29524500	8.61098600	3.29543800
H	1.50864500	9.31436500	1.69033300
H	-0.92187600	9.97117700	1.66804900
H	-0.90541300	8.79006500	4.48824400
H	-2.25676300	9.64620700	3.73294300
N	-0.77626300	6.89144800	2.40494700
O	-0.92168100	5.60146500	2.33270100
C	-2.59534700	6.84386400	4.06285700
H	-3.34860200	7.46478400	4.55671800
H	-3.09324200	5.95177800	3.67551400
H	-1.85860000	6.53627400	4.81089700
C	-2.97724100	7.94123300	1.82818200
H	-3.31476700	7.00829300	1.36919400
H	-3.84721300	8.42970400	2.27797300
H	-2.59911500	8.60247400	1.04636000
C	1.58919900	6.48968000	1.84732100
H	1.42618900	5.55939400	1.29924000
H	2.49155700	6.96261700	1.44847300
H	1.76284100	6.24817200	2.90013800
C	0.08942900	7.64380700	0.18386100
H	0.99927900	7.97019800	-0.33036200
H	-0.22682900	6.69801100	-0.26574500
H	-0.68185000	8.39559400	0.00368900
N	0.00803600	10.99931100	3.15705200
C	-0.79275800	12.11060700	3.02236200
C	-0.28342000	13.38120000	3.67599700
H	-0.21372100	14.16298300	2.91390200
H	-1.01429800	13.71699500	4.41818600
H	0.69130900	13.26885100	4.16020200
O	-1.84541700	12.06123500	2.39785700
H	0.80858600	11.03146300	3.77335800
H	-0.14163700	2.45643600	-0.92874800

Oxetane Cation

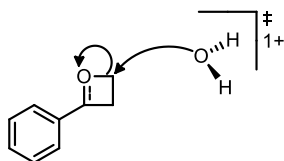


Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-4.30923900	1.26715700	1.38225400
C	-2.92523200	1.32558400	1.16079900
C	-2.37095100	2.45826900	0.58849500
C	-3.21249100	3.54465500	0.23424800
C	-4.61337800	3.47614500	0.46211900
C	-5.15028900	2.33685600	1.03499400

H	-4.73900700	0.37649900	1.83154200
H	-2.29379400	0.48780500	1.43685700
H	-1.30103500	2.51719600	0.41121900
H	-5.24622900	4.31367700	0.18665400
H	-6.21785700	2.26909800	1.21585500
C	-2.64076300	4.69268500	-0.34780900
C	-1.27707500	5.17058500	-0.74935800
C	-2.05145300	6.43316400	-1.19195800
H	-0.80080700	4.59328200	-1.54744300
H	-0.57171100	5.30305100	0.07634300
H	-1.89774900	7.34673200	-0.61852400
O	-3.30335100	5.76027900	-0.72091300
H	-2.13042700	6.62858500	-2.26089600

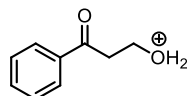
Oxetane TS2



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-4.62624500	1.30080200	1.32428900
C	-3.23718300	1.32321100	1.15605500
C	-2.62634700	2.44808800	0.61529100
C	-3.40843500	3.55881900	0.23967500
C	-4.80827100	3.52851300	0.41253200
C	-5.41004200	2.40057000	0.95347000
H	-5.10117400	0.42053800	1.74756800
H	-2.63895500	0.46585800	1.44730800
H	-1.54738900	2.46474300	0.48659700
H	-5.39711900	4.39141900	0.11906700
H	-6.48648100	2.37167400	1.08897200
C	-2.79414000	4.74180300	-0.32365100
C	-1.32493100	4.96659800	-0.58651400
C	-1.48900400	6.37530100	-1.14127100
H	-0.90057200	4.26764500	-1.31546300
H	-0.70128100	4.94768400	0.31248700
H	-1.59968100	7.20752600	-0.45922000
O	-3.41260100	5.77290400	-0.68027900
H	-1.79515800	6.53569400	-2.16637600
O	0.34149900	6.76508700	-1.43492900
H	0.69288200	6.38292600	-2.26105500
H	0.50135200	7.72640400	-1.48785000

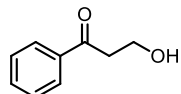
Oxetane H2O Cation



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-3.15268000	-1.94237900	0.04007800
C	-1.83293800	-1.60184200	-0.21139100
C	-1.45780800	-0.23713800	-0.30819000
C	-2.44626200	0.77048200	-0.14276500
C	-3.75967700	0.41698500	0.11457700
C	-4.11380400	-0.93665000	0.20555800
H	-3.43902500	-2.98642400	0.11066400
H	-1.10174300	-2.39178400	-0.33973400
H	-2.16296400	1.81392800	-0.21961200
H	-4.51354300	1.18663300	0.24330800
H	-5.14572500	-1.20938300	0.40669400
C	-0.10718000	0.14861500	-0.58568700
C	1.03639500	-0.80819400	-0.81880400
C	2.39760100	-0.26362100	-0.36691600
H	0.85208600	-1.76635800	-0.33106000
H	1.07459300	-1.00111000	-1.90201900
H	3.17967500	-0.98642500	-0.61810000
O	0.14623900	1.41364500	-0.68012600
H	2.40990900	-0.09144700	0.71682600
O	2.60364600	0.96972500	-1.08222500
H	3.40825800	1.41604300	-0.76904400
H	1.13243200	1.55775400	-0.88210000

3a Oxetane Product

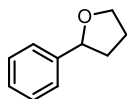


Coordinates (from last standard orientation):

ATOM	X	Y	Z
0 1			
C	-4.31179700	1.38208100	1.53934900
C	-2.92506900	1.54181200	1.51444200
C	-2.35621600	2.58993800	0.79196800
C	-3.17063500	3.48725000	0.08350600
C	-4.56437300	3.31390200	0.11154500
C	-5.13119300	2.27068200	0.83628900
H	-4.75389500	0.56617300	2.10494000
H	-2.28660200	0.85083900	2.05776100
H	-1.27661500	2.70027300	0.77904100
H	-5.18076900	4.01264800	-0.44434600
H	-6.21040300	2.14630500	0.85432600
C	-2.61517600	4.62349500	-0.71513800
C	-1.11054900	4.86680900	-0.73385600
H	-0.72037400	4.84557500	0.29261600
H	-0.63327700	4.03220700	-1.26715500
C	-0.73685200	6.18871600	-1.41610200

H	0.35044800	6.31440900	-1.38666200
H	-1.18122800	7.02479300	-0.85280700
O	-1.11322000	6.22350300	-2.77877900
H	-2.08510300	6.16970200	-2.76699800
O	-3.36734700	5.35186000	-1.35778300

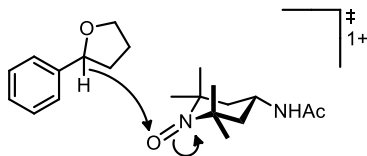
2e Furan SM



Coordinates (from last standard orientation):

ATOM	X	Y	Z
0 1			
C	-5.37358800	1.50943900	0.75270900
C	-5.74351800	2.63501600	0.01398900
C	-4.81041100	3.63564100	-0.26033400
C	-3.49488200	3.52393600	0.20324400
C	-3.13425100	2.39849500	0.95396000
C	-4.06419700	1.39398700	1.22337900
H	-6.10205100	0.73195500	0.96749600
H	-6.76415800	2.73745900	-0.34623700
H	-5.09652900	4.52136100	-0.81796900
H	-2.11825900	2.30942000	1.33422500
H	-3.76859000	0.52641900	1.80783800
C	-2.45221600	4.56912200	-0.13280300
O	-3.06372600	5.84359100	-0.36628000
C	-1.64405900	4.27715300	-1.41302800
C	-2.38654900	6.54162700	-1.42041500
C	-1.17603800	5.68099400	-1.81476200
H	-2.30739900	3.85248800	-2.17580600
H	-0.82679800	3.57019600	-1.24092000
H	-3.08114400	6.66898400	-2.26282300
H	-2.10201700	7.53856100	-1.06281700
H	-0.92346100	5.76961800	-2.87598000
H	-0.29214300	5.96940300	-1.23346000
H	-1.75446500	4.65800200	0.71706700

Furan TSI

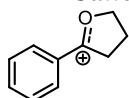


Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
H	-2.01576500	5.67710600	0.62110800
C	-2.71269100	7.02491000	3.24274600
C	-2.19307700	8.63758900	1.17521800
C	-2.32118300	9.81679800	2.16960800
C	-3.26754500	9.53992700	3.33541200
C	-2.77158900	8.30672700	4.10287800

H	-1.32197700	10.04684600	2.56570400
H	-2.65357800	10.69428200	1.60458000
H	-4.28169500	9.35146500	2.97221800
H	-1.77284800	8.51656100	4.50780500
H	-3.43834100	8.11445300	4.94829700
N	-2.01950600	7.36345200	1.95204000
O	-1.37676300	6.40979300	1.36020500
C	-1.88241500	5.95494600	3.96861000
H	-2.30188300	5.81215500	4.96882400
H	-1.90966400	4.99313700	3.45091700
H	-0.83889700	6.26607500	4.07456300
C	-4.13617000	6.47757600	2.97577600
H	-4.10760900	5.61110800	2.31106300
H	-4.56393600	6.15849900	3.93143200
H	-4.80870100	7.22596400	2.55260000
C	-0.94237100	8.85419700	0.30760000
H	-0.87574800	8.12743500	-0.50472700
H	-0.99621900	9.85217500	-0.13779900
H	-0.02880200	8.79373900	0.90646000
C	-3.43977300	8.53522900	0.26282400
H	-3.48554200	9.43053000	-0.36583400
H	-3.37100300	7.66492100	-0.39653400
H	-4.37272500	8.47659300	0.82693400
N	-3.38329000	10.70750200	4.19378800
C	-4.50157900	10.88511700	4.97652300
C	-4.49998100	12.11229600	5.86843100
H	-3.60467200	12.73249400	5.76422100
H	-5.38063700	12.71724100	5.63300600
H	-4.59503000	11.79423500	6.91124100
O	-5.43773200	10.09650800	4.93333600
H	-2.57840300	11.30384100	4.32937300
C	-5.61142900	2.63494200	1.24353600
C	-5.81559500	3.59576300	0.24725900
C	-4.73697700	4.29745000	-0.28030200
C	-3.43096200	4.03306700	0.18158600
C	-3.23533500	3.07131200	1.19629000
C	-4.31997800	2.37391900	1.71545900
H	-6.45681900	2.08807300	1.65020700
H	-6.81749000	3.79062800	-0.12268000
H	-4.88836000	5.02898100	-1.06620600
H	-2.23513100	2.86156800	1.56403800
H	-4.16173800	1.62341500	2.48370000
C	-2.27490000	4.74722400	-0.37754500
O	-2.51922600	5.50066400	-1.47964800
C	-0.87850700	4.13713100	-0.48564300
C	-1.32176900	5.62238200	-2.30865500
C	-0.16970000	5.11110300	-1.44117200
H	-0.97518600	3.13418500	-0.92212100
H	-0.37772600	4.03555700	0.47981800
H	-1.49740400	5.00270500	-3.19406200
H	-1.24154400	6.66705200	-2.61406600
H	0.60814700	4.62731900	-2.03604500
H	0.28697400	5.92966200	-0.87800900

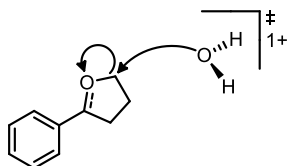
THF Cation



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-5.36504100	1.58449700	1.04311700
C	-5.88395900	2.83644300	0.68074400
C	-5.06428100	3.77397800	0.07600200
C	-3.70136100	3.46178200	-0.17165400
C	-3.18932200	2.19324400	0.20173300
C	-4.02224200	1.26317100	0.80318100
H	-6.01328500	0.85352300	1.51764000
H	-6.92590600	3.06954200	0.87361900
H	-5.45343600	4.74499800	-0.20994400
H	-2.14934900	1.94440200	0.01777500
H	-3.63505500	0.29096900	1.08929800
C	-2.84713200	4.41393200	-0.79811500
O	-3.32079100	5.56804700	-1.14433900
C	-1.39787800	4.27288900	-1.16827100
C	-2.29514000	6.40342600	-1.81954000
C	-0.97317600	5.72825300	-1.45677200
H	-1.33588700	3.63670700	-2.06360100
H	-0.81019500	3.78583100	-0.38672600
H	-2.54425800	6.37054400	-2.88295500
H	-2.43472900	7.41301000	-1.43500000
H	-0.24312400	5.79836100	-2.26515200
H	-0.53900600	6.18396700	-0.56271000

THF TS2

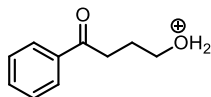


Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-5.32646400	1.38883200	1.10610600
C	-5.85572700	2.68317900	1.07095000
C	-5.11701400	3.72010300	0.51392900
C	-3.83466700	3.47514700	-0.01263600
C	-3.31120600	2.16982900	0.02769000
C	-4.05619600	1.13307200	0.58322700
H	-5.90453100	0.57882600	1.54140100
H	-6.84318100	2.87866300	1.47787800
H	-5.51127000	4.72995100	0.47674700
H	-2.32663100	1.95096500	-0.37425400
H	-3.64769700	0.12757200	0.61044300
C	-3.09455300	4.61384300	-0.59678000
O	-3.57441100	5.74510500	-0.65351200

C	-1.68870100	4.38504000	-1.16819400
C	-1.66280000	6.50750900	-2.53527700
C	-0.94759100	5.70502100	-1.47752000
H	-1.76101700	3.76096300	-2.06959200
H	-1.07646000	3.81754500	-0.45973100
H	-1.75641500	6.00735300	-3.49943100
H	-2.58940300	6.96299200	-2.19579300
H	0.06495000	5.46580800	-1.82069800
H	-0.88033800	6.29254800	-0.55356300
O	-0.70368000	7.70969300	-2.91744300
H	-0.43458400	8.22135500	-2.12384300
H	-1.10935300	8.32850300	-3.56265900

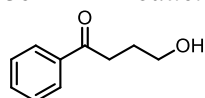
THF H2O Cation



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-3.15274800	-1.82728000	-0.52399500
C	-1.81611400	-1.50192000	-0.34680200
C	-1.44712700	-0.18685600	0.03199400
C	-2.46315500	0.78669100	0.22351400
C	-3.79407000	0.45211400	0.03717900
C	-4.14058100	-0.85335800	-0.33603400
H	-3.42994400	-2.83614800	-0.81127200
H	-1.06881000	-2.27244500	-0.49555100
H	-2.18734300	1.79381800	0.51332800
H	-4.56631300	1.20072300	0.18087100
H	-5.18522800	-1.11244400	-0.48177000
C	-0.07283200	0.19121900	0.24117500
C	1.09427600	-0.75254600	0.08225700
C	2.40261000	-0.16376700	-0.50904700
H	1.29231700	-1.17260100	1.08189400
H	0.78509300	-1.59516900	-0.53594500
C	3.29706400	0.59901200	0.45960400
H	2.98769100	-1.00839700	-0.88780700
H	2.18022600	0.46972600	-1.37578000
H	3.51705200	-0.00225400	1.35077900
O	0.14084500	1.40190100	0.61663200
H	4.23958000	0.86171400	-0.03073800
O	2.61327200	1.81506200	0.83832700
H	3.06356100	2.26199600	1.57353200
H	1.13769800	1.63273900	0.77254000

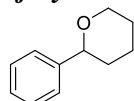
3e THF Product



Coordinates (from last standard orientation):

ATOM	X	Y	Z
0 1			
C	-3.56806200	0.89892200	1.63436500
C	-4.06480400	2.13277200	2.06546600
C	-3.55372000	3.31252100	1.53394500
C	-2.53946200	3.27736600	0.56343700
C	-2.04744500	2.03434200	0.13686000
C	-2.55942500	0.85172100	0.67036800
H	-3.96653600	-0.02323800	2.04909200
H	-4.85004500	2.17122300	2.81559700
H	-3.92332700	4.28133800	1.85363200
H	-1.26317100	1.98097600	-0.61163800
H	-2.17122600	-0.10561000	0.33365400
C	-2.02852000	4.58441100	0.03146000
O	-2.48187400	5.64172000	0.44359600
C	-0.92850000	4.56968300	-1.02812000
C	0.62913800	5.94581000	-2.49514400
C	-0.53896500	5.96840000	-1.50876100
H	-1.26242700	3.95074300	-1.87335500
H	-0.05498900	4.04641300	-0.61034800
H	1.50889500	5.46853500	-2.02881500
H	0.37335600	5.34967600	-3.37864600
H	-0.27752100	6.58637400	-0.63954400
H	-1.39829200	6.45626900	-1.98142400
O	0.95186600	7.23755200	-2.99477900
H	1.18084600	7.79410000	-2.23399800

2j Pyran SM

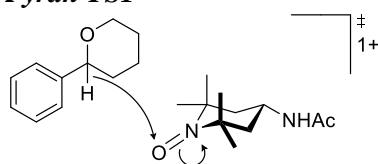


Coordinates (from last standard orientation):

ATOM	X	Y	Z
0 1			
C	-3.36162400	0.53803100	0.79301400
C	-1.96792900	0.48100000	0.76580900
C	-1.22806600	1.40952000	0.02373300
C	-1.90899400	2.40462500	-0.68710300
C	-3.30294200	2.46625000	-0.65604200
C	-4.03418200	1.53281400	0.08068400
H	-3.92086000	-0.18860400	1.37684400
H	-1.44908600	-0.29005400	1.33239100
H	-1.33702900	3.13571300	-1.24834800
H	-3.81895300	3.24820800	-1.20758200
H	-5.11961400	1.58323300	0.10471800
C	0.28144200	1.29581100	-0.03885400
C	0.74675500	0.29935700	-1.12039700

H	0.65285000	0.93898800	0.93953000
C	2.27965300	0.27246800	-1.21661900
H	0.31260400	0.61166500	-2.07922100
H	0.34838200	-0.69738600	-0.89467000
C	2.24879100	2.60492100	-0.29185600
C	2.82534600	1.69815200	-1.38023600
H	2.60076500	-0.36622300	-2.04833500
H	2.69453400	-0.17196300	-0.29968900
H	2.53539100	3.65014400	-0.44419500
H	2.62516800	2.29124700	0.69812400
H	3.92186500	1.71039600	-1.33171600
H	2.53607600	2.09669500	-2.36154500
O	0.82575500	2.59105300	-0.28897700

Pyran TS1

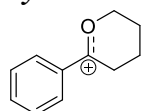


Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
H	-2.11950000	5.66382100	1.22278700
C	-0.09665500	7.41172400	2.81870600
C	-2.64802800	8.23195600	2.77083500
C	-2.08973500	9.66445100	2.64013400
C	-0.73347700	9.85703500	3.31480600
C	0.27889700	8.89781800	2.67386700
H	-1.99626900	9.91123000	1.57283900
H	-2.83223900	10.34898200	3.06503500
H	-0.80087800	9.64039300	4.38522300
H	0.37479800	9.14888800	1.60877600
H	1.25823000	9.04539400	3.13774200
N	-1.55571000	7.23421200	2.48539700
O	-1.95237700	6.00746800	2.34406300
C	0.74097500	6.57665100	1.83816900
H	1.79814100	6.80892200	1.99657100
H	0.60503800	5.50554900	2.00611000
H	0.48610100	6.82035400	0.80255600
C	0.14921100	6.89365800	4.25679000
H	-0.21400000	5.86692200	4.35887100
H	1.22500600	6.90331000	4.45719100
H	-0.33233800	7.51460000	5.01479000
C	-3.77291700	8.03370700	1.74139400
H	-4.26900300	7.06959600	1.86843800
H	-4.52028700	8.82008100	1.88495300
H	-3.38650800	8.10735700	0.72095500
C	-3.20465100	7.96241200	4.18931300
H	-4.08820800	8.58856700	4.34940800
H	-3.50292000	6.91502700	4.28756600
H	-2.48130800	8.19549200	4.97393200
N	-0.30167000	11.24301000	3.22350700
C	0.63531700	11.73689600	4.10090400

C	1.01874600	13.19340000	3.91790200
H	0.75448500	13.74245200	4.82705600
H	2.10435100	13.26246600	3.80224500
H	0.53552000	13.67423500	3.06190300
O	1.11078600	11.03099200	4.98176100
H	-0.62148600	11.81394400	2.45362400
C	-5.63719000	3.69735600	0.57467000
C	-4.27078200	3.94002600	0.62424000
C	-3.70427500	4.99382300	-0.12898300
C	-4.55395500	5.81399700	-0.90317900
C	-5.91885800	5.55561200	-0.95800500
C	-6.46447500	4.49992500	-0.22038400
H	-6.06225700	2.88366900	1.15402500
H	-3.64188700	3.32044800	1.25640200
H	-4.12848300	6.63171900	-1.47339000
H	-6.56031000	6.17500300	-1.57747700
H	-7.53153400	4.30297300	-0.26246400
C	-2.24945400	5.23955900	-0.09718100
C	-1.27592200	4.06627900	-0.14627600
C	-0.69114800	3.92257600	-1.56737500
C	-1.03919200	6.37501000	-1.91657300
C	-0.02755800	5.24264700	-1.96667100
H	-1.48671000	3.66078000	-2.27658800
H	0.03278400	3.10195300	-1.57505400
H	-1.75672000	6.29446000	-2.74298200
H	-0.57510700	7.36177800	-1.95264100
O	-1.84939000	6.39866600	-0.69454800
H	0.37521400	5.19348500	-2.98518800
H	0.81611900	5.45426200	-1.29841300
H	-0.44807500	4.23844700	0.54920400
H	-1.78152100	3.15046300	0.16465000

Pyran Cation

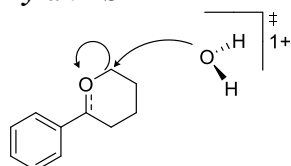


Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-3.41847500	0.31470300	0.03760400
C	-2.05000600	0.24944000	-0.17692600
C	-1.28809000	1.44060100	-0.27311500
C	-1.94064500	2.69402500	-0.14451500
C	-3.30749000	2.74632500	0.07437400
C	-4.04713200	1.55952700	0.16506600
H	-3.99916200	-0.59903100	0.10875000
H	-1.57806800	-0.72174000	-0.27403800
H	-1.36422300	3.60871400	-0.21790500
H	-3.80378700	3.70604800	0.17448300
H	-5.11858400	1.60516200	0.33680400
C	0.13157600	1.38826700	-0.51120600
C	0.89345900	0.10224800	-0.67905200
C	2.41973400	0.25922600	-0.63961700
H	0.57705300	-0.31264700	-1.64886700

H	0.54816600	-0.61194200	0.07473800
C	2.17761400	2.72024500	-0.84360600
C	2.83331300	1.49466400	-1.44170000
H	2.88200200	-0.64517300	-1.04344800
H	2.75912600	0.35417400	0.39888500
H	2.20881800	3.60159200	-1.48486900
H	2.57653300	2.97687500	0.14148300
H	3.91798100	1.64370100	-1.41512300
H	2.54846700	1.38715900	-2.49553300
O	0.72405900	2.53093900	-0.60745700

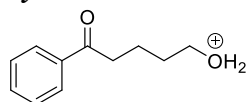
Pyran TS2



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-3.18917300	-1.88717800	-0.40573900
C	-1.84250800	-1.53994100	-0.34723900
C	-1.46438400	-0.22268900	-0.02605900
C	-2.46204700	0.73723800	0.23247100
C	-3.80508100	0.38774000	0.16627600
C	-4.17006800	-0.92477000	-0.15212900
H	-3.47483500	-2.90530400	-0.65131400
H	-1.09373500	-2.29986200	-0.54645500
H	-2.16255400	1.75047600	0.47759400
H	-4.57008500	1.13322300	0.36083400
H	-5.22023600	-1.19725700	-0.20359800
C	-0.04982500	0.18869400	0.05858600
C	1.06438700	-0.79341200	-0.26838200
C	2.40912100	1.83397200	1.19881800
C	2.43077900	-0.12850300	-0.45434500
H	1.10547800	-1.55754700	0.52191400
H	0.80942300	-1.33377200	-1.18686600
C	3.05615300	0.53571300	0.79762200
H	1.68246200	1.86442300	1.99904100
H	2.28203700	2.59377100	0.43674700
H	3.13829600	-0.89783500	-0.77963700
H	2.37762200	0.60966900	-1.26264900
H	4.10216200	0.75476300	0.55161900
H	3.05079200	-0.16720900	1.63950900
O	0.25669200	1.33967700	0.39848200
O	3.73953900	2.65357400	2.02689500
H	4.06021000	2.14603700	2.79867600
H	3.47214900	3.53635700	2.35269600

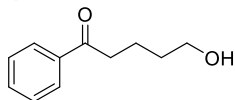
Pyran h2o Cation



Coordinates (from last standard orientation):

ATOM	X	Y	Z
1 1			
C	-2.95907500	-1.25631000	-0.73148400
C	-1.63719100	-1.26595600	-0.31036900
C	-1.09152200	-0.13558600	0.34679700
C	-1.91444900	0.99986500	0.56841900
C	-3.23423100	0.99611000	0.14905400
C	-3.75754400	-0.13023800	-0.50072400
H	-3.37218300	-2.12289500	-1.23703200
H	-1.03315200	-2.14529400	-0.50036900
H	-1.50151300	1.86575000	1.07270300
H	-3.86161300	1.86400300	0.32409000
H	-4.79323300	-0.12983200	-0.82789700
C	0.27703500	-0.10726200	0.79157200
C	1.25339000	-1.23751900	0.65535300
C	3.97908400	0.70858000	0.74663300
C	2.35317300	-0.95540100	-0.43281300
H	1.73059100	-1.38084300	1.63230100
H	0.72855600	-2.16284700	0.42571000
C	3.76287100	-0.65622800	0.10845000
H	3.72281800	1.52120400	0.05450700
H	5.02607800	0.82030400	1.04269400
H	2.41781100	-1.85168300	-1.05622500
H	2.02971100	-0.14929700	-1.10360600
H	4.46451900	-0.71887000	-0.73271600
H	4.06127600	-1.43460100	0.82127000
O	0.69446800	0.99126800	1.32150500
O	3.15425500	0.81786600	1.94279200
H	3.48277000	1.54221700	2.50127500
H	1.68573100	0.94938900	1.61847900

3j Pyran h2o Cation



Coordinates (from last standard orientation):

ATOM	X	Y	Z
0 1			
C	-3.21413900	0.19536800	0.60442000
C	-1.85769400	0.11680100	0.28771100
C	-1.15239200	1.26310500	-0.11026900
C	-1.83470700	2.48873800	-0.18523400
C	-3.18755800	2.56689000	0.12827300
C	-3.88084800	1.41891300	0.52474100
H	-3.74986800	-0.69873600	0.91139900
H	-1.35558300	-0.84323400	0.35283600
H	-1.27577800	3.36581000	-0.49455800
H	-3.70501500	3.52040400	0.06539100
H	-4.93796900	1.47865900	0.77004900
C	0.30748600	1.25194700	-0.46194500
C	1.11179400	-0.03688200	-0.33453600
H	0.53259500	-0.90591500	-0.66822900

H	1.97354600	0.06626400	-1.00125700
C	1.60539700	-0.25877400	1.11125600
H	2.18038300	0.62411700	1.42060500
H	0.74454200	-0.32259900	1.79062700
C	2.46785500	-1.51882900	1.24792000
H	1.89326600	-2.40633100	0.95121500
H	3.32952600	-1.46219600	0.57050900
C	2.98228200	-1.73231300	2.66633900
H	3.59302000	-0.86741200	2.97491300
H	2.13185800	-1.79750600	3.36626200
O	0.86508600	2.28221800	-0.81371800
O	3.74791700	-2.93267200	2.67563700
H	4.09104200	-3.06062100	3.57276300