

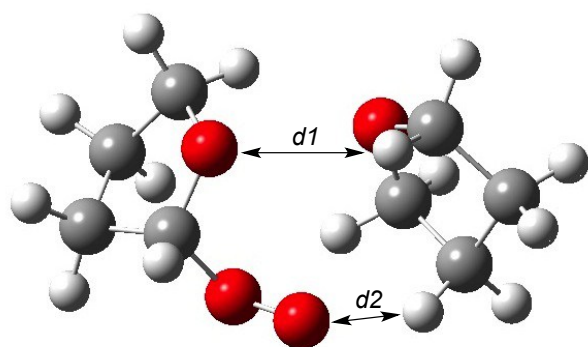
Supplementary Materials

An *ab-initio* and DFT study of the autoxidation of THF and THP

Hiroshi Matsubara,* Syouhei Suzuki and Shun Hirano

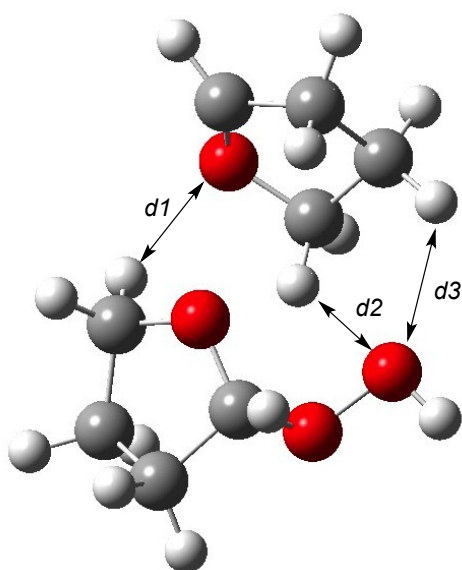
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Figures S1–S6, Table S1, a full list of reference 10 and HF/6-311G**, MP2/6-311G**, MP2/cc-pVDZ, BHandHLYP/6-311G**, BHandHLYP/cc-pVDZ, B3LYP/6-311G**, B3LYP/cc-pVDZ, MPW1K/cc-pVDZ, MPWKIS1K/cc-pVDZ, and M05/cc-pVDZ Gaussian Archive entries for the optimized structures in this study and higher-level calculated single-point energies.



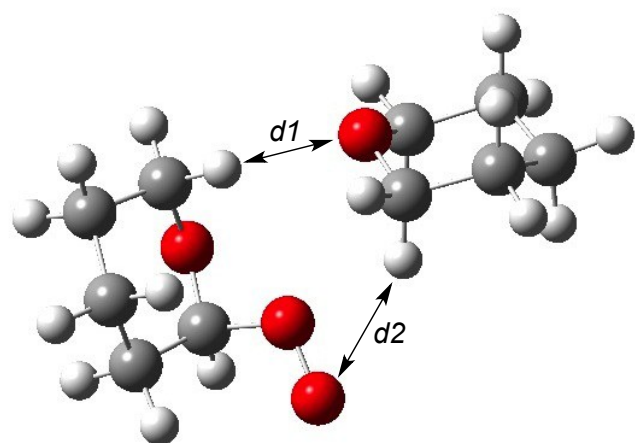
	<i>d1</i> (Å)	<i>d2</i> (Å)
HF/6-311G**	2.596	2.922
MP2/6-311G**	2.503	2.565
MP2/cc-pVDZ	2.506	2.529
BHandHLYP/6-311G**	2.374	2.575
BhandHLYP/cc-pVDZ	2.505	2.553
B3LYP/6-311G**	2.392	2.586
B3LYP/cc-pVDZ	2.363	2.502
MPW1K/cc-pVDZ	2.358	2.559
MPWKCIS1/cc-pVDZ	2.392	2.570
M05/cc-pVDZ	2.575	2.530

Figure S1 Optimized geometry of complex **5a**



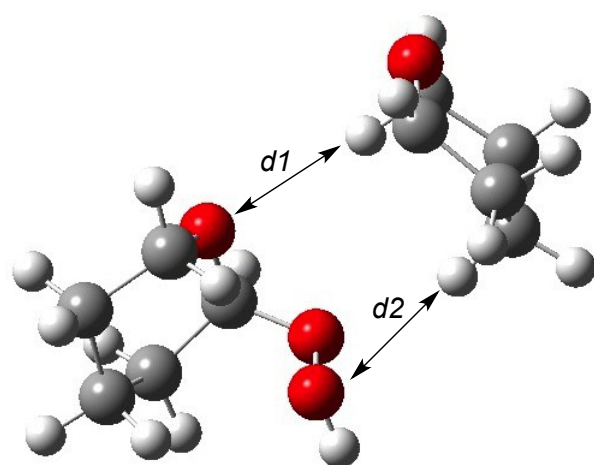
	<i>d1</i> (Å)	<i>d2</i> (Å)	<i>d3</i> (Å)
HF/6-311G**	2.844	2.853	3.133
MP2/6-311G**	2.782	2.714	2.673
MP2/cc-pVDZ	2.702	2.702	2.637
BHandHLYP/6-311G**	2.571	2.728	2.740
BhandHLYP/cc-pVDZ	2.764	2.757	2.665
B3LYP/6-311G**	2.878	2.910	2.773
B3LYP/cc-pVDZ	2.785	2.864	2.685
MPW1K/cc-pVDZ	2.548	2.752	2.756
MPWKCIS1/cc-pVDZ	2.634	2.850	2.751
M05/cc-pVDZ	2.817	2.825	2.641

Figure S2 Optimized geometry of complex **7a**



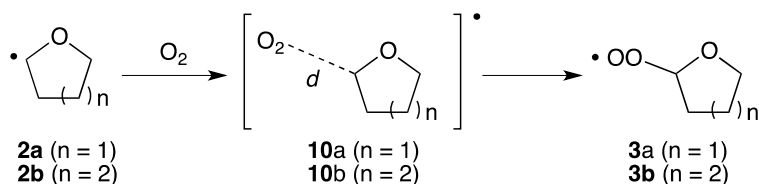
	<i>d1</i> (Å)	<i>d2</i> (Å)
HF/6-311G**	2.704	2.936
BHandHLYP/6-311G**	2.833	2.632
BhandHLYP/cc-pVDZ	2.397	2.595
MPW1K/cc-pVDZ	2.405	2.643

Figure S3 Optimized geometry of complex **5b**



	<i>d1</i> (Å)	<i>d2</i> (Å)
HF/6-311G**	2.833	2.930
BHandHLYP/6-311G**	2.542	2.669
BhandHLYP/cc-pVDZ	2.521	2.640
MPW1K/cc-pVDZ	2.541	2.693

Figure S4 Optimized geometry of complex **7b**



Scheme S1 Reaction pathway for radical coupling process of the first cycle of autoxidation of THF and THP.

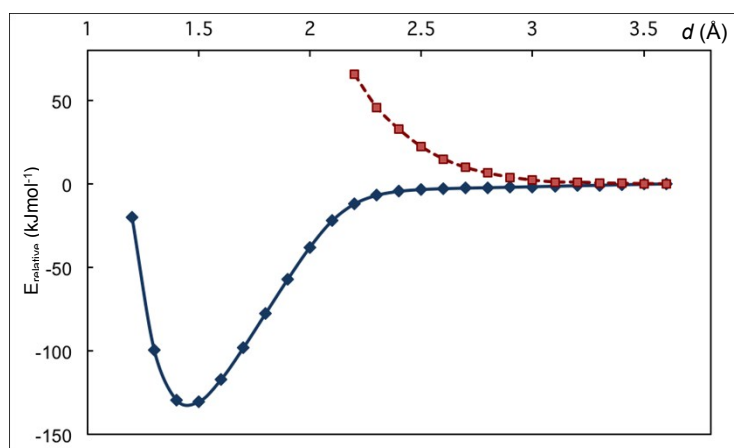


Figure S5 BHandHLYP/6-311G** calculated dependence of the energy of complex **10a** on distance (d) in the radical coupling process of complex **10a** involving THF radical (**2a**) with molecular oxygen (Scheme S1). Solid line: calculation in the doublet state; dotted line: calculation in the quartet state. No energy barriers are found when d is shortend.

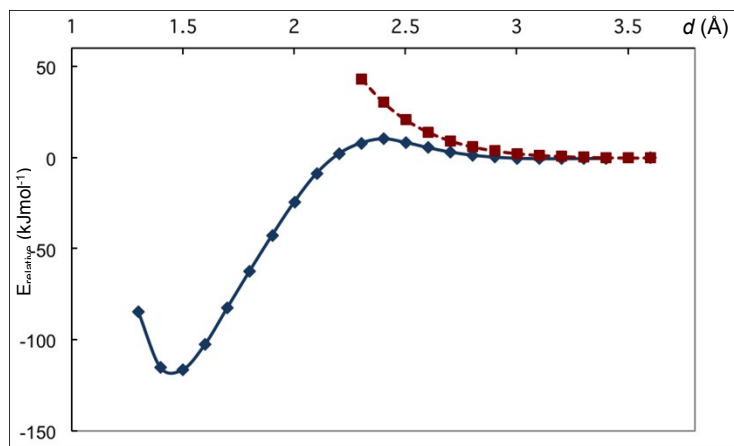
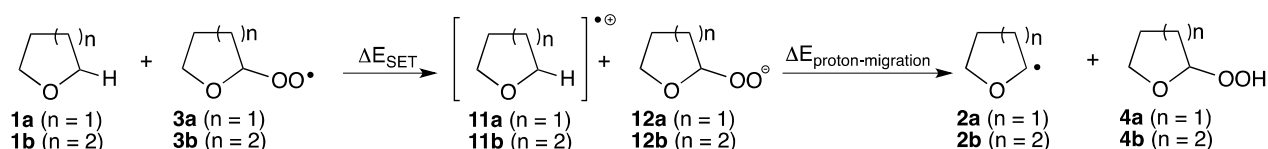


Figure S6 BHandHLYP/6-311G** calculated dependence of the energy of complex **10b** on distance (d) in the radical coupling process of complex **10b** involving THP radical (**2b**) with molecular oxygen (Scheme S1). Solid line: calculation in the doublet state; dotted line: calculation in the quartet state. Energy barriers of 10.5 kJmol^{-1} exist around $d = 2.4 \text{ Å}$.



Scheme S2 Mechanisms of hydrogen transfer involving SET and proton migration.

Table S1 BHandHLYP/6-311G** calculated reaction energies (in kJmol⁻¹) for SET and proton migration (Scheme S2)

	ΔE_{SET}	$\Delta E_{\text{proton-migration}}$
THF	796.6 (358.9)	-753.1 (-330.0)
THP	780.6 (370.6)	-721.6 (-325.3)

Energies including solvent effect (calculated by the PCM method, solvent = THF) are listed in parenthesis.

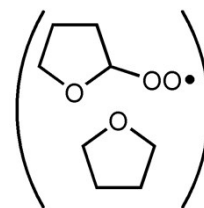
Full list of Reference 10

Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, 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, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Gaussian 09, Revision C.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, T. Keith, 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, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

Gaussian Archive entries

Complex of THF and tetrahydrofuran-2-peroxyl radical (5a)



HF/6-311G**

1\1\GINC-I7\FOpt\UHF\6-311G(d,p)\C8H15O4(2)\SUZUKI\30-May-2011\1\#HF/6-311G** OPT=(z-matrix,readFC,Maxcycle=150,Maxstep=15) NoSymm freq=NoRaman geom=check guess=read\THF-THF radical complex HF/6-311G**\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\H,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\O,14,r14,13,a14,4,d14,0\C,15,r15,14,a15,13,d15,0\C,16,r16,15,a16,14,d16,0\C,17,r17,16,a17,15,d17,0\C,18,r18,17,a18,16,d18,0\O,19,r19,18,a19,17,d19,0\H,16,r20,15,a20,17,d20,0\H,17,r21,16,a21,18,d21,0\H,17,r22,16,a22,18,d22,0\H,18,r23,17,a23,19,d23,0\H,18,r24,17,a24,19,d24,0\H,19,r25,18,a25,20,d25,0\H,19,r26,18,a26,20,d26,0\|r1=1.52567161|r2=1.5291112|r3=1.52779539|r4=1.4144804|r5=1.08839007|r6=1.0836848|r7=1.08417888|r8=1.08505113|r9=1.08677067|r10=1.08362867|r11=1.08407052|r12=1.08518506|r13=3.21240569|r14=1.29360154|r15=1.42617013|r16=1.51685061|r17=1.53136588|r18=1.53147511|r19=1.42613776|r20=1.0792769|r21=1.08156061|r22=1.0852114|r23=1.08363846|r24=1.08293393|r25=1.08440353|r26=1.07957569|a2=101.30836407|a3=101.62277413|a4=106.09255831|a5=111.08512185|a6=113.22156465|a7=113.67453743|a8=110.23970736|a9=110.52732507|a10=112.52186652|a11=108.85586979|a12=108.96099903|a13=131.67188121|a14=95.07073057|a15=111.63976026|a16=106.54684778|a17=101.22637197|a18=102.24192247|a19=105.91341998|a20=107.13647431|a21=112.40382213|a22=108.61575476|a23=110.11828987|a24=113.20711752|a25=111.93395622|a26=112.99311508|d3=36.16139661|d4=-29.1047736|d5=118.65135391|d6=-119.31915096|d7=121.14727112|d8=-116.8821665|d9=117.07482508|d10=-121.81855327|d11=121.90364557|d12=-119.92349409|d13=70.63161845|d14=-88.00818458|d15=-76.57395648|d16=-172.91413649|d17=-84.47115107|d18=-32.7244514|d19=21.76192456|d20=125.16712043|d21=122.48542002|d22=-116.97638863|d23=117.4296844|d24=-121.16309056|d25=-116.83735621|d26=119.18159661\|Version=EM64L-G03RevE.01\HF=-611.1419298\S2=0.760352\S2-1=0.\S2A=0.750076\RMSD=3.758e-09\RMSF=3.055e-06\Thermal=0.\Dipole=-0.3695547,0.4003433,-0.3989617\PG=C01 [X(C8H15O4)]\@

MP2/6-311G**

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QCISD=-613.1826451

CCSD(T)/6-311G**//MP2/cc-pVDZ

CCSD(T)=-613.250971

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=-612.9731892

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)=-613.0289009

BHandHLYP/6-311G**

1\1\GINC-I7\FOptUBHandHLYP\6-311G(d,p)\C8H15O4(2)\SUZUKI\30-May-2011\1\#BHandHLYP/6-311G** OPT=(z-matrix,readFC,Maxcycle=150,Maxstep=15) NoSymm freq=NoRaman geom=check guess=read\THF-THFo radical complex BHandHLYP/6-311G**\|0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\H,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\O,14,r14,13,a14,4,d14,0\C,15,r15,14,a15,13,d15,0\C,16,r16,15,a16,14,d16,0\C,17,r17,16,a17,15,d17,0\C,18,r18,17,a18,16,d18,0\O,19,r19,18,a19,17,d19,0\H,16,r20,15,a20,17,d20,0\H,17,r21,16,a21,18,d21,0\H,17,r22,16,a22,18,d22,0\H,18,r23,17,a23,19,d23,0\H,18,r24,17,a24,19,d24,0\H,19,r25,18,a25,20,d25,0\H,19,r26,18,a26,20,d26,0\|r1=1.52213404\r2=1.52496519\r3=1.52066752\r4=1.42244721\r5=1.08956986\r6=1.08527932\r7=1.08444629\r8=1.08485172\r9=1.08709685\r10=1.08400001\r11=1.08528782\r12=1.08688472\r13=2.8446537\r14=1.29444732\r15=1.45338661\r16=1.51120035\r17=1.5273622\r18=1.52545213\r19=1.4366198\r20=1.08125767\r21=1.08232398\r22=1.0855093\r23=1.08414035\r24=1.08315095\r25=1.08559544\r26=1.08066843\|a2=101.66907741\|a3=101.60014598\|a4=105.92102313\|a5=111.29959238\|a6=112.82253473\|a7=113.4917684\|a8=110.00522432\|a9=110.52746931\|a10=112.53565308\|a11=108.48824863\|a12=109.06038015\|a13=128.92419152\|a14=92.79547027\|a15=111.58349192\|a16=106.08349967\|a17=101.2322361\|a18=102.52963275\|a19=105.88833498\|a20=105.83125105\|a21=112.31793379\|a22=108.61011387\|a23=110.07770568\|a24=113.08439438\|a25=112.23267071\|a26=112.63029447\|d3=36.55521483\|d4=-31.65858118\|d5=118.57627694\|d6=-119.36096073\|d7=121.10367842\|d8=-116.96464414\|d9=117.24853552\|d10=-121.49970572\|d11=121.72455755\|d12=-120.02427266\|d13=63.02430225\|d14=-81.4414318\|d15=-77.07731828\|d16=-169.48262712\|d17=-84.27381481\|d18=-32.60158732\|d19=21.75998517\|d20=125.36209493\|d21=122.34860024\|d22=-117.22723916\|d23=117.24654858\|d24=-121.38377851\|d25=-116.64393786\|d26=118.375552

3\\Version=EM64L-G03RevE.01\\HF=-614.4343558\\S2=0.75609\\S2-1=0.\\S2A=0.750022\\RMSD=4.361e-09\\RMSF=7.766e-06\\Thermal=0.\\Dipole=-0.3186801,0.4015486,-0.6196221\\PG=C01[X(C8H15O4)]\\@

BHandHLYP/cc-pVDZ

1\\GINC-I7FOptUBHandHLYP\\CC-pVDZ\\C8H15O4(2)\\SUZUKI\\01-Jun-2011\\I\\#BHandHLYP/cc-pVDZ OPT=(z-matrix,readFC,Maxcycle=150,Maxstep=15) NoSymm freq=NoRaman geom=check guess=read\\THF-THFooradical complex BHandHLYP/cc-pVDZ\\0,2\\C\\C,1,r1\\C,2,r2,1,a2\\C,3,r3,2,a3,1,d3,0\\O,4,r4,3,a4,2,d4,0\\H,1,r5,2,a5,5,d5,0\\H,1,r6,2,a6,5,d6,0\\H,2,r7,3,a7,1,d7,0\\H,2,r8,3,a8,1,d8,0\\H,3,r9,4,a9,2,d9,0\\H,3,r10,4,a10,2,d10,0\\H,4,r11,5,a11,3,d11,0\\H,4,r12,5,a12,3,d12,0\\O,13,r13,4,a13,5,d13,0\\O,14,r14,13,a14,4,d14,0\\C,15,r15,14,a15,13,d15,0\\C,16,r16,15,a16,14,d16,0\\C,17,r17,16,a17,15,d17,0\\C,18,r18,17,a18,16,d18,0\\O,19,r19,18,a19,17,d19,0\\H,16,r20,15,a20,17,d20,0\\H,17,r21,16,a21,18,d21,0\\H,17,r22,16,a22,18,d22,0\\H,18,r23,17,a23,19,d23,0\\H,18,r24,17,a24,19,d24,0\\H,19,r25,18,a25,20,d25,0\\H,19,r26,18,a26,20,d26,0\\r1=1.52290067\\r2=1.52496474\\r3=1.52035335\\r4=1.42093028\\r5=1.09806738\\r6=1.09322875\\r7=1.0922518\\r8=1.09268931\\r9=1.09519788\\r10=1.09199073\\r11=1.09377564\\r12=1.09560179\\r13=2.75190844\\r14=1.2956076\\r15=1.4513126\\r16=1.51257088\\r17=1.52665631\\r18=1.52188725\\r19=1.43341197\\r20=1.08967011\\r21=1.09028877\\r22=1.09350041\\r23=1.09148198\\r24=1.0911038\\r25=1.09497084\\r26=1.08860477\\a2=101.69649441\\a3=101.39651045\\a4=105.90086096\\a5=111.43608862\\a6=112.57216651\\a7=113.65769877\\a8=109.92239049\\a9=110.43873366\\a10=112.65781367\\a11=108.49698478\\a12=109.27188531\\a13=127.55454236\\a14=86.50719138\\a15=111.20144643\\a16=106.48316345\\a17=101.3543272\\a18=102.15308761\\a19=105.91461433\\a20=105.48379898\\a21=112.06850486\\a22=108.69449447\\a23=110.32046519\\a24=113.29534042\\a25=112.3414243\\a26=112.33011446\\d3=36.66234625\\d4=-32.78856771\\d5=118.68394007\\d6=-119.35223094\\d7=121.30286719\\d8=-116.64152784\\d9=117.19206661\\d10=-121.67452046\\d11=121.75633547\\d12=-120.15844294\\d13=53.94897289\\d14=-69.14034985\\d15=-84.97976671\\d16=-167.83148524\\d17=-86.33026425\\d18=-33.63400353\\d19=25.13754158\\d20=125.13983552\\d21=122.50850986\\d22=-117.36344371\\d23=116.28761432\\d24=-121.52461092\\d25=-117.17228423\\d26=118.55622681\\Version=EM64L-G03RevE.01\\HF=-614.3106525\\S2=0.755683\\S2-1=0.\\S2A=0.75002\\RMSD=8.070e-09\\RMSF=7.083e-06\\Thermal=0.\\Dipole=-0.2107453,0.2085301,-0.7170223\\PG=C01 [X(C8H15O4)]\\@

BHandHLYP/aug-cc-pVDZ//BHandHLYP/cc-pVDZ

HF=-614.3524437

B3LYP/6-311G**

1\\GINC-I7FOptUB3LYP\\6-311G(d,p)\\C8H15O4(2)\\SUZUKI\\30-May-2011\\I\\#B3LYP/6-311G** OPT=(z-matrix,readFC,Maxcycle=150,Maxstep=15) NoSymm freq=NoRaman geom=check guess=read\\THF-THFooradical complex B3LYP/6-311G**\\0,2\\C\\C,1,r1\\C,2,r2,1,a2\\C,3,r3,2,a3,1,d3,0\\O,4,r4,3,a4,2,d4,0\\H,1,r5,2,a5,5,d5,0\\H,1,r6,2,a6,5,d6,0\\H,2,r7,3,a7,1,d7,0\\H,2,r8,3,a8,1,d8,0\\H,3,r9,4,a9,2,d9,0\\H,3,r10,4,a10,2,d10,0\\H,4,r11,5,a11,3,d11,0\\H,4,r12,5,a12,3,d12,0\\O,13,r13,4,a13,5,d13,0\\O,14,r14,13,a14,4,d14,0\\C,15,r15,14,a15,13,d15,0\\C,16,r16,15,a16,14,d16,0\\C,17,r17,16,a17,15,d17,0\\C,18,r18,17,a18,16,d18,0\\O,19,r19,18,a19,17,d19,0\\H,16,r20,15,a20,17,d20,0\\H,17,r21,16,a21,18,d21,0\\H,17,r22,16,a22,18,d22,0\\H,18,r23,17,a23,19,d23,0\\H,18,r24,17,a24,19,d24,0\\H,19,r25,18,a25,20,d25,0\\H,19,r26,18,a26,20,d26,0\\r1=1.53231772\\r2=1.53569387\\r3=1.529371\\r4=1.4409896\\r5=1.09780226\\r6=1.09350938\\r7=1.09209271\\r8=1.09255935\\r9=1.09461529\\r10=1.09167075\\r11=1.09323814\\r12=1.09524489\\r13=2.99225822\\r14=1.31689291\\r15=1.49481288\\r16=1.5199374\\r17=1.53923081\\r18=1.53649094\\r19=1.45823206\\r20=1.08901955\\r21=1.09000362\\r22=1.09308113\\r23=1.09144618\\r24=1.09064496\\r25=1.09306051\\r26=1.08927949\\a2=101.87815929\\a3=101.63265238\\a4=105.9471492\\a5=111.44945321\\a6=112.77249989\\a7=113.32799228\\a8=110.01407669\\a9=110.60826638\\a10=112.52810689\\a11=108.14521234\\a12=109.1055008\\a13=128.20260746\\a14=92.95702923\\a15=111.37619956\\a16=105.62285637\\a17=101.40553267\\a18=102.93238693\\a19=106.00159819\\a20=104.91695682\\a21=112.39315265\\a22=108.59216573\\a23=109.96098583\\a24=112.83811704\\a25=112.50608206\\a26=113.06036872\\d3=36.70184394\\d4=-32.65916848\\d5=118.48541004\\d6=-119.37068838\\d7=121.08321391\\d8=-117.1544226\\d9=117.41707049\\d10=-121.27536836\\d11=121.76381113\\d12=-119.97853447\\d13=64.25214159\\d14=-85.95973306\\d15=-73.58934724\\d16=-168.02470063\\d17=-83.97786592\\d18=-31.121016\\d19=19.3599611\\d20=125.68530885\\d21=122.2088368\\d22=-117.52224807\\d23=117.61706594\\d24=-121.41289116\\d25=-116.28110102\\d26=118.14815832\\Version=EM64L-G03RevE.01\\HF=-614.7958433\\S2=0.753504\\S2-1=0.\\S2A=0.750008\\RMSD=4.447e-09\\RMSF=3.001e-05\\Thermal=0.\\Dipole=-0.2497356,0.51292,-0.6856577\\PG=C01 [X(C8H15O4)]\\@

B3LYP/cc-pVDZ

1\\GINC-I7FOptUB3LYP\\CC-pVDZ\\C8H15O4(2)\\SUZUKI\\01-Jun-2011\\I\\#B3LYP/cc-pVDZ OPT=(z-matrix,readFC,Maxcycle=150,Maxstep=15) NoSymm freq=NoRaman geom=check guess=read\\THF-THFooradical complex B3LYP/cc-pVDZ\\0,2\\C\\C

.46558031\ a12=109.54393587\ a13=128.99855368\ a14=94.5334071\ a15=111.25411903\ a16=106.29353983\ a17=101.09557806\ a18=102.478189\ a19=106.17375439\ a20=105.55452768\ a21=112.37685508\ a22=108.55229095\ a23=109.96395384\ a24=113.31088097\ a25=112.16168362\ a26=112.87709206\ d3=36.75960714\ d4=-33.98536089\ d5=118.8638502\ d6=-120.00688081\ d7=121.415351\ d8=-116.96513934\ d9=117.22221088\ d10=-121.67407165\ d11=121.968716\ d12=-120.05198837\ d13=63.89332506\ d14=-84.63050236\ d15=-73.24929944\ d16=-169.66012666\ d17=-83.88852935\ d18=-32.76246824\ d19=21.69048431\ d20=125.41849519\ d21=122.51646051\ d22=-117.40409504\ d23=117.41916631\ d24=-121.69339442\ d25=-116.98290871\ d26=118.81776768\ \Version=EM64L-G03RevE.01\HF=-614.2637397\ S2=0.754392\ S2-1=0.\ S2A=0.750012\ RMSD=2.708e-09\ RMSF=1.294e-05\ Thermal=0.\ Dipole=-0.2837747,0.4773878,-0.6134243\ PG=C01 [X(C8H15O4)]\ \@

M05/cc-pVDZ

1\ \GINC-I7\FOpt\UM05\CC-pVDZ\C8H15O4(2)\SUZUKI\07-Jun-2011\1\ \#M05/cc-pVDZ scf=qc OPT=(z-matrix,readFC,Maxcycle=100) NoSymm freq=NoRaman geom=check guess=read\ \THF-THFooradical complex M05/cc-pVDZ\ \0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\H,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\O,14,r14,13,a14,4,d14,0\C,15,r15,14,a15,13,d15,0\C,16,r16,15,a16,14,d16,0\C,17,r17,16,a17,15,d17,0\C,18,r18,17,a18,16,d18,0\O,19,r19,18,a19,17,d19,0\H,16,r20,15,a20,17,d20,0\H,17,r21,16,a21,18,d21,0\H,17,r22,16,a22,18,d22,0\H,18,r23,17,a23,19,d23,0\H,18,r24,17,a24,19,d24,0\H,19,r25,18,a25,20,d25,0\H,19,r26,18,a26,20,d26,0\ r1=1.5215156\ r2=1.52282622\ r3=1.51937334\ r4=1.42184211\ r5=1.10607054\ r6=1.10099406\ r7=1.09755989\ r8=1.09848434\ r9=1.10092925\ r10=1.09743364\ r11=1.10152351\ r12=1.10434763\ r13=2.6805093\ r14=1.29008848\ r15=1.48800961\ r16=1.51050285\ r17=1.52418337\ r18=1.51913281\ r19=1.43682338\ r20=1.09755601\ r21=1.09591984\ r22=1.0993166\ r23=1.09740225\ r24=1.09640038\ r25=1.10248198\ r26=1.09607131\ a2=101.58739421\ a3=101.3077099\ a4=106.02364743\ a5=111.37452611\ a6=112.56951576\ a7=113.65834393\ a8=109.86414266\ a9=110.47956454\ a10=112.6793482\ a11=108.56669533\ a12=109.5148906\ a13=127.21064445\ a14=86.24134494\ a15=111.54980643\ a16=106.13625248\ a17=101.2984364\ a18=102.07606602\ a19=106.05748877\ a20=104.284909\ a21=112.20977742\ a22=108.60119993\ a23=110.28955829\ a24=113.37879674\ a25=112.43074425\ a26=112.58080089\ d3=37.00022394\ d4=-33.0833178\ d5=118.9902705\ d6=-119.43484446\ d7=121.30948421\ d8=-116.59646616\ d9=117.24818857\ d10=-121.62989945\ d11=121.79746567\ d12=-120.29750159\ d13=52.4661865\ d14=-67.04998821\ d15=-85.99240191\ d16=-167.89441297\ d17=-86.63780154\ d18=-33.75585294\ d19=25.80716102\ d20=125.08361149\ d21=122.59172576\ d22=-117.49168761\ d23=116.07282591\ d24=-121.58635497\ d25=-117.28433432\ d26=118.67075703\ \Version=EM64L-G03RevE.01\HF=-614.2707263\ S2=0.753568\ S2-1=0.\ S2A=0.75001\ RMSD=8.975e-09\ RMSF=3.503e-05\ Thermal=0.\ Dipole=-0.1575316,0.1842903,-0.8145667\ PG=C01 [X(C8H15O4)]\ \@

G3(MP2)-RAD//MP2/cc-pVDZ

G3=-614.0344859

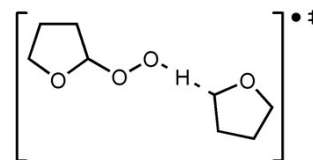
G3(MP2)-RAD//B3LYP/6-31G*

G3=-614.0335567

Transition state involved in the abstraction of α -hydrogen in THF (6a)

HF/6-311G**

1\ \GINC-I7\FTS\UHF\6-311G(d,p)\C8H15O4(2)\SUZUKI\13-May-2011\1\ \#HF/6-311G** OPT=(TS,NoEigenTest,z-matrix,CalcFC,Maxcycle=100) NoSymm\ \THFTS HF/6-311G**\ \0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\O,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\X,14,1,13,90,4,0,0\H,14,r14,15,a14,13,d14,0\X,16,1,14,90,15,0,0\C,16,r15,17,a15,14,d15,0\C,18,r16,16,a16,17,d16,0\C,19,r17,18,a17,16,d17,0\C,20,r18,19,a18,18,d18,0\O,21,r19,20,a19,19,d19,0\H,18,r20,19,a20,22,d20,0\H,19,r21,20,a21,18,d21,0\H,19,r22,20,a22,18,d22,0\H,20,r23,21,a23,19,d23,0\H,20,r24,21,a24,19,d24,0\H,21,r25,22,a25,20,d25,0\H,21,r26,22,a26,20,d26,0\ r1=1.52540789\ r2=1.53719513\ r3=1.53664954\ r4=1.37909218\ r5=1.08099705\ r6=1.08712441\ r7=1.08492202\ r8=1.08368956\ r9=1.0824735\ r10=1.08293163\ r11=1.0790512\ r12=1.40277217\ r13=1.3569532\ r14=1.21361685\ r15=1.3134924\ r16=1.52897152\ r17=1.53783806\ r18=1.52418405\ r19=1.41350011\ r20=1.08049244\ r21=1.08411541\ r22=1.08368041\ r23=1.08328517\ r24=1.08506691\ r25=1.08582164\ r26=1.08099718\ a2=101.92643448\ a3=103.58711535\ a4=107.02347611\ a5=114.23675657\ a6=111.48729927\ a7=110.65195038\ a8=113.1119343\ a9=111.32086856\ a10=109.16047058\ a11=108.02098818\ a12=111.89333471\ a13=110.40751866\ a14=93.5267664\ a15=92.36610785\ a16=107.2073311\ a17=102.56562144\ a18=102.07182416\ a19=104.20263



262\a20=118.35894772\ a21=111.41805627\ a22=112.75596116\ a23=112.81592322\ a24=109.82242481\ a25=109.62408307\ a26=107.84114174\ d3=-18.96384084\ d4=-3.06249792\ d5=117.43597352\ d6=-118.65656585\ d7=116.66959492\ d8=-121.69031066\ d9=121.5710095\ d10=-119.21716696\ d11=124.5320391\ d12=-116.11482399\ d13=-67.34428274\ d14=103.86962451\ d15=174.96772823\ d16=168.01827221\ d17=119.91126873\ d18=-22.89121837\ d19=35.17344521\ d20=-127.95396825\ d21=118.10497327\ d22=-120.55783581\ d23=121.80677881\ d24=-117.21800135\ d25=119.4415794\ d26=-121.75001289\ \Version=EM64L-G03RevE.01\HF=-611.0795065\ S2=0.797069\ S2-1=0.\ S2A=0.750764\ RMSD=5.824e-09\ RMSF=1.132e-05\ Thermal=0.\ Dipole=0.5710102,0.3630961,0.9551323\ PG=C01[X(C8H15O4)]\ \@

MP2/6-311G**

1\ \GINC-I7\FTS\UMP2-FC\6-311G(d,p)\C8H15O4(2)\SUZUKI\18-May-2011\I\#MP2/6-311G** OPT=(TS,NoEigenTest,z-matrix,CalcFC,Maxcycle=100) NoSymm geom=check guess=read\ \THF TS MP2/6-311G**\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\O,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\X,14,1.,13,90.,4,0.,0\H,14,r14,15,a14,13,d14,0\X,16,1.,14,90.,15,0.,0\C,16,r15,17,a15,14,d15,0\C,18,r16,16,a16,17,d16,0\C,19,r17,18,a17,16,d17,0\C,20,r18,19,a18,18,d18,0\O,21,r19,20,a19,19,d19,0\H,18,r20,19,a20,22,d20,0\H,19,r21,20,a21,18,d21,0\H,19,r22,20,a22,18,d22,0\H,20,r23,21,a23,19,d23,0\H,20,r24,21,a24,19,d24,0\H,21,r25,22,a25,20,d25,0\H,21,r26,22,a26,20,d26,0\ r1=1.52639087\ r2=1.53701087\ r3=1.53846309\ r4=1.39655728\ r5=1.09071501\ r6=1.09760914\ r7=1.09334045\ r8=1.0926884\ r9=1.09149115\ r10=1.09365052\ r11=1.08980815\ r12=1.4321463\ r13=1.37388427\ r14=1.27617614\ r15=1.23558126\ r16=1.53482451\ r17=1.53774073\ r18=1.52365024\ r19=1.43602069\ r20=1.09284867\ r21=1.09401819\ r22=1.0926298\ r23=1.0925372\ r24=1.09362398\ r25=1.0961306\ r26=1.09119402\ a2=101.09911031\ a3=103.19652822\ a4=107.69122338\ a5=114.69018321\ a6=111.14773647\ a7=110.59543413\ a8=113.19377306\ a9=111.46556906\ a10=108.52629003\ a11=107.99417439\ a12=112.19784381\ a13=109.45856525\ a14=88.14235422\ a15=93.20336181\ a16=106.99476643\ a17=102.33759136\ a18=101.11909783\ a19=103.7092433\ a20=117.60423287\ a21=110.52476744\ a22=113.12096245\ a23=113.08295375\ a24=109.48175643\ a25=109.7375984\ a26=107.16607715\ d3=-22.72226493\ d4=-1.66807715\ d5=116.70836763\ d6=-118.31266523\ d7=115.61041003\ d8=-121.6038279\ d9=122.51451181\ d10=-118.01461014\ d11=126.1142595\ d12=-114.79837875\ d13=-69.42812404\ d14=102.8290122\ d15=166.62143817\ d16=166.99150441\ d17=121.43005475\ d18=-27.6583102\ d19=40.6077466\ d20=-125.69851314\ d21=117.11214856\ d22=-121.02281026\ d23=121.32640164\ d24=-116.62337965\ d25=118.84529225\ d26=-121.65423305\ \Version=EM64L-G03RevE.01\HF=-611.0781082\ MP2=-613.0388776\ PUHF=-611.0872886\ PMP2-0=-613.0452048\ S2=0.790228\ S2-1=0.764946\ S2A=0.750747\ RMSD=7.142e-09\ RMSF=1.067e-05\ Thermal=0.\ Dipole=0.4404594,0.324294,0.9587086\ PG=C01[X(C8H15O4)]\ \@

MP2/cc-pVDZ

1\ \GINC-I7\FTS\UMP2-FC\CC-pVDZ\C8H15O4(2)\SUZUKI\17-May-2011\I\#MP2/cc-pVDZ OPT=(TS,NoEigenTest,z-matrix,readFC,Maxcycle=100) NoSymm geom=check guess=read\ \THF TS MP2/cc-pVDZ\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\O,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\X,14,1.,13,90.,4,0.,0\H,14,r14,15,a14,13,d14,0\X,16,1.,14,90.,15,0.,0\C,16,r15,17,a15,14,d15,0\C,18,r16,16,a16,17,d16,0\C,19,r17,18,a17,16,d17,0\C,20,r18,19,a18,18,d18,0\O,21,r19,20,a19,19,d19,0\H,18,r20,19,a20,22,d20,0\H,19,r21,20,a21,18,d21,0\H,19,r22,20,a22,18,d22,0\H,20,r23,21,a23,19,d23,0\H,20,r24,21,a24,19,d24,0\H,21,r25,22,a25,20,d25,0\H,21,r26,22,a26,20,d26,0\ r1=1.5302659\ r2=1.54020413\ r3=1.54261199\ r4=1.40060258\ r5=1.09957487\ r6=1.10713551\ r7=1.10252891\ r8=1.1013622\ r9=1.10004273\ r10=1.10239708\ r11=1.09857892\ r12=1.43523324\ r13=1.38111203\ r14=1.27849733\ r15=1.24347157\ r16=1.53724713\ r17=1.54035637\ r18=1.52723363\ r19=1.43967149\ r20=1.1021957\ r21=1.10304763\ r22=1.10113619\ r23=1.10116771\ r24=1.10282712\ r25=1.10515591\ r26=1.10021773\ a2=101.07867109\ a3=103.24713523\ a4=107.761832486\ a5=114.74195939\ a6=111.1008634\ a7=110.7098783\ a8=113.31367957\ a9=111.56970887\ a10=108.52063183\ a11=107.99310167\ a12=112.34768782\ a13=109.08427247\ a14=88.86221223\ a15=93.77524451\ a16=106.97053243\ a17=102.34422902\ a18=101.02979024\ a19=103.82017883\ a20=117.78253562\ a21=110.56633061\ a22=113.40271058\ a23=113.13994395\ a24=109.64819268\ a25=109.91408736\ a26=107.2247204\ d3=-22.68309386\ d4=-1.71815404\ d5=116.98974496\ d6=-118.53701904\ d7=115.76434332\ d8=-121.71577731\ d9=122.5921294\ d10=-118.16076461\ d11=126.19769309\ d12=-114.72318283\ d13=-69.49574714\ d14=102.06275514\ d15=165.34812233\ d16=170.04449696\ d17=123.2830175\ d18=-28.63415461\ d19=40.54822691\ d20=-125.98925364\ d21=116.92784104\ d22=-121.30953762\ d23=121.43976968\ d24=-116.70548202\ d25=118.97513961\ d26=-121.76570651\ \Version=EM64L-G03RevE.01\HF=-610.9663321\ MP2=-612.8169908\ PUHF=-610.9755239\ PMP2-0=-612.8233517\ S2=0.790815\ S2-1=0.765397\ S2A=0.750758\ RMSD=9.599e-09\ RMSF=2.038e-05\ Thermal=0.\ Dipole=0.427862,0.3237953,0.9544129\ PG=C01 [X(C8H15O4)]\ \@

MP2/aug-cc-pVDZ//MP2/cc-pVDZ

MP2=-612.953531

QCISD/6-311G//MP2/cc-pVDZ**

QCISD=-613.1447787

CCSD(T)/6-311G//MP2/cc-pVDZ**

CCSD(T)=-613.2170106

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=-612.9347397

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)=-612.9940418

BHandHLYP/6-311G**

1\1\GINC-I7\FTS\UBHandHLYP\6-311G(d,p)\C8H15O4(2)\SUZUKI\16-May-2011\1\#BHandHLYP/6-311G** OPT=(TS,NoEigenTest,z-matrix,CalcFC,Maxcycle=100) NoSymm geom=check guess=read\THF TS BHandHLYP/6-311G**\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\O,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\X,14,1,13,90,4,0,0\H,14,r14,15,a14,13,d14,0\X,16,1,14,90,15,0,0\C,16,r15,17,a15,14,d15,0\C,18,r16,16,a16,17,d16,0\C,19,r17,18,a17,16,d17,0\C,20,r18,19,a18,18,d18,0\O,21,r19,20,a19,19,d19,0\H,18,r20,19,a20,22,d20,0\H,19,r21,20,a21,18,d21,0\H,19,r22,20,a22,18,d22,0\H,20,r23,21,a23,19,d23,0\H,20,r24,21,a24,19,d24,0\H,21,r25,22,a25,20,d25,0\H,21,r26,22,a26,20,d26,0\|1=1.52067348\|2=1.53203251\|3=1.53254052\|4=1.38477204\|5=1.08211883\|6=1.0887722\|7=1.08524297\|8=1.0839926\|9=1.08260565\|10=1.08411953\|11=1.08164031\|12=1.41332794\|13=1.37460747\|14=1.22060592\|15=1.29652323\|16=1.52264035\|17=1.53381858\|18=1.51911344\|19=1.42359555\|20=1.08257881\|21=1.0853261\|22=1.08433433\|23=1.08348293\|24=1.08536179\|25=1.08671344\|26=1.08205547\|a2=101.90789574\|a3=103.64902224\|a4=107.2119033\|a5=114.42817149\|a6=111.43875436\|a7=110.64106674\|a8=113.0846934\|a9=111.44296383\|a10=108.77921844\|a11=107.91866183\|a12=112.10795253\|a13=109.96781411\|a14=92.35523974\|a15=93.68620048\|a16=106.57946932\|a17=102.75731392\|a18=102.1996653\|a19=104.13747535\|a20=118.90999675\|a21=111.31570085\|a22=112.7007694\|a23=112.69531897\|a24=109.89576377\|a25=109.15763294\|a26=107.52226793\|d3=-20.00042465\|d4=-2.46766466\|d5=117.23926063\|d6=-118.58241724\|d7=116.6207195\|d8=-121.69451326\|d9=121.96761908\|d10=-118.95163717\|d11=125.24323869\|d12=-115.6113868\|d13=-67.42650121\|d14=103.45023228\|d15=171.70418754\|d16=165.47577416\|d17=117.64473492\|d18=-22.67370354\|d19=35.29791378\|d20=-128.37256455\|d21=118.01597963\|d22=-120.83808924\|d23=121.7412011\|d24=-117.29996103\|d25=119.4423444\|d26=-121.83203294\|Version=EM64L-G03RevE.01\HF=-614.3959955\S2=0.764952\S2-1=0.S2A=0.750094\RMSD=2.770e-09\RMSF=2.375e-05\Thermal=0.\Dipole=0.5885281,0.3440963,1.0021688\PG=C01 [X(C8H15O4)]\@@

BHandHLYP/cc-pVDZ

1\1\GINC-I7\FTS\UBHandHLYP\CC-pVDZ\C8H15O4(2)\SUZUKI\17-May-2011\1\#BHandHLYP/cc-pVDZ OPT=(TS,NoEigenTest,z-matrix,readFC,Maxcycle=100) NoSymm geom=check guess=read\THF TS BHandHLYP/cc-pVDZ\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\O,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\X,14,1,13,90,4,0,0\H,14,r14,15,a14,13,d14,0\X,16,1,14,90,15,0,0\C,16,r15,17,a15,14,d15,0\C,18,r16,16,a16,17,d16,0\C,19,r17,18,a17,16,d17,0\C,20,r18,19,a18,18,d18,0\O,21,r19,20,a19,19,d19,0\H,18,r20,19,a20,22,d20,0\H,19,r21,20,a21,18,d21,0\H,19,r22,20,a22,18,d22,0\H,20,r23,21,a23,19,d23,0\H,20,r24,21,a24,19,d24,0\H,21,r25,22,a25,20,d25,0\H,21,r26,22,a26,20,d26,0\|1=1.52123689\|2=1.53210479\|3=1.53293883\|4=1.38640413\|5=1.09040883\|6=1.0972818\|7=1.09342072\|8=1.09189552\|9=1.09041019\|10=1.09215714\|11=1.08966796\|12=1.41390804\|13=1.37652239\|14=1.2178528\|15=1.304838\|16=1.52252534\|17=1.53325095\|18=1.51935313\|19=1.42369278\|20=1.09110921\|21=1.09360525\|22=1.09216682\|23=1.09142478\|24=1.09357734\|25=1.09485811\|26=1.09040375\|a2=101.84777706\|a3=103.61543123\|a4=107.24699077\|a5=114.42646375\|a6=111.35560866\|a7=110.67695482\|a8=113.18101227\|a9=111.56753715\|a10=108.65722321\|a11=107.89728739\|a12=112.04944609\|a13=109.63189768\|a14=92.26206421\|a15=93.95182944\|a16=106.59208768\|a17=102.71016101\|a18=102.10736478\|a19=104.23746183\|a20=119.07518563\|a21=111.26106657\|a22=112.93877718\|a23=112.

7367676\ a24=109.90338119\ a25=109.23822339\ a26=107.52949375\ d3=-20.15841291\ d4=-2.38355251\ d5=117.37847069\ d6=-118.73842724\ d7=116.61636845\ d8=-121.76595289\ d9=122.10058958\ d10=-118.88753924\ d11=125.31099407\ d12=-115.57121326\ d13=-66.54903024\ d14=102.90446225\ d15=170.367616\ d16=168.0775941\ d17=118.93222477\ d18=-23.65550121\ d19=35.57507892\ d20=-128.57963826\ d21=117.75633662\ d22=-121.06650141\ d23=121.84575729\ d24=-117.26904093\ d25=119.49081277\ d26=-121.86897648\ \Version=EM64L-G03RevE.01\HF=-614.272209\ S2=0.7648\ S2-1=0.\ S2A=0.750088\ RMSD=6.839e-09\ RMSF=2892e-05\ Thermal=0.\ Dipole=0.5799665,0.314775,0.9825632\ PG=C01 [X(C8H15O4)]\ \@

BHandHLYP/aug-cc-pVDZ//BHandHLYP/cc-pVDZ
HF=-614.3165845

B3LYP/6-311G**

1\1\GINC-I7\FTS\UB3LYP\6-311G(d,p)\C8H15O4(2)\SUZUKI\16-May-2011\1\#B3LYP/6-311G** OPT=(TS,NoEigenTest,z-matrix,CalcFC,Maxcycle=100) NoSymm geom=check guess=read\THF TS B3LYP/6-311G**\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\O,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\X,14,1,13,90,4,0,0\H,14,r14,15,a14,13,d14,0\X,16,1,14,90,15,0,0\C,16,r15,17,a15,14,d15,0\C,18,r16,16,a16,17,d16,0\C,19,r17,18,a17,16,d17,0\C,20,r18,19,a18,18,d18,0\O,21,r19,20,a19,19,d19,0\H,18,r20,19,a20,22,d20,0\H,19,r21,20,a21,18,d21,0\H,19,r22,20,a22,18,d22,0\H,20,r23,21,a23,19,d23,0\H,20,r24,21,a24,19,d24,0\H,21,r25,22,a25,20,d25,0\H,21,r26,22,a26,20,d26,0\ r1=1.53051832\ r2=1.54194569\ r3=1.54375365\ r4=1.40091318\ r5=1.08997316\ r6=1.09698176\ r7=1.09280738\ r8=1.09172269\ r9=1.0901487\ r10=1.09197701\ r11=1.08989209\ r12=1.43483887\ r13=1.408002\ r14=1.21805996\ r15=1.32619495\ r16=1.53039336\ r17=1.54518514\ r18=1.52862739\ r19=1.44402943\ r20=1.09063211\ r21=1.09331714\ r22=1.0922419\ r23=1.09106551\ r24=1.09290775\ r25=1.09440497\ r26=1.08980892\ a2=101.99950261\ a3=103.74971449\ a4=107.32986415\ a5=114.54237741\ a6=111.49974571\ a7=110.63966168\ a8=112.99659422\ a9=111.41036336\ a10=108.74543745\ a11=107.57346214\ a12=112.49918033\ a13=109.66629167\ a14=94.56017942\ a15=94.08126261\ a16=106.38103652\ a17=102.95176874\ a18=102.37123416\ a19=104.24005829\ a20=119.31620192\ a21=111.22623924\ a22=112.60379114\ a23=112.55082335\ a24=110.01448129\ a25=108.8617369\ a26=107.12158102\ d3=-20.57915752\ d4=-1.85011075\ d5=116.92018703\ d6=-118.65244806\ d7=116.73725138\ d8=-121.65904021\ d9=122.10246686\ d10=-118.90131669\ d11=125.68311164\ d12=-115.33753102\ d13=-68.19083491\ d14=103.60301987\ d15=174.06411181\ d16=164.83467734\ d17=117.13170671\ d18=-22.45168847\ d19=34.84553284\ d20=-128.42979951\ d21=118.1048405\ d22=-121.01708065\ d23=121.64030345\ d24=-117.49576578\ d25=119.62081911\ d26=-121.93121582\ \Version=EM64L-G03RevE.01\HF=-614.768956\ S2=0.75599\ S2-1=0.\ S2A=0.75002\ RMSD=8.408e-09\ RMSF=3.472e-05\ Thermal=0.\ Dipole=0.5983984,0.3725707,1.0310259\ PG=C01 [X(C8H15O4)]\ \@

B3LYP/cc-pVDZ

1\1\GINC-I7\FTS\UB3LYP\CC-pVDZ\C8H15O4(2)\SUZUKI\17-May-2011\1\#B3LYP/cc-pVDZ OPT=(TS,NoEigenTest,z-matrix,readFC,Maxcycle=100) NoSymm geom=check guess=read\THF TS B3LYP/cc-pVDZ\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\O,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\X,14,1,13,90,4,0,0\H,14,r14,15,a14,13,d14,0\X,16,1,14,90,15,0,0\C,16,r15,17,a15,14,d15,0\C,18,r16,16,a16,17,d16,0\C,19,r17,18,a17,16,d17,0\C,20,r18,19,a18,18,d18,0\O,21,r19,20,a19,19,d19,0\H,18,r20,19,a20,22,d20,0\H,19,r21,20,a21,18,d21,0\H,19,r22,20,a22,18,d22,0\H,20,r23,21,a23,19,d23,0\H,20,r24,21,a24,19,d24,0\H,21,r25,22,a25,20,d25,0\H,21,r26,22,a26,20,d26,0\ r1=1.53138445\ r2=1.54219184\ r3=1.54436946\ r4=1.40253342\ r5=1.09908109\ r6=1.10655035\ r7=1.10173214\ r8=1.10034534\ r9=1.09866514\ r10=1.1007795\ r11=1.09892683\ r12=1.4350655\ r13=1.40809115\ r14=1.21073875\ r15=1.33962627\ r16=1.53046175\ r17=1.54454892\ r18=1.52918981\ r19=1.44325041\ r20=1.09989465\ r21=1.10240306\ r22=1.10080505\ r23=1.09970615\ r24=1.10186041\ r25=1.10347674\ r26=1.0989764\ a2=101.87737946\ a3=103.6838318\ a4=107.37465924\ a5=114.55400644\ a6=111.35665051\ a7=110.7039147\ a8=113.09196366\ a9=111.54776275\ a10=108.61300008\ a11=107.51315682\ a12=112.44630507\ a13=109.3160295\ a14=93.87864385\ a15=94.64612612\ a16=106.21740585\ a17=102.87249072\ a18=102.23423707\ a19=104.35180534\ a20=119.57553383\ a21=111.18023978\ a22=112.87131158\ a23=112.58367504\ a24=110.01294498\ a25=108.92533223\ a26=107.140246\ d3=-20.82107946\ d4=-1.73883228\ d5=117.09548693\ d6=-118.84482361\ d7=116.73345681\ d8=-121.67942537\ d9=122.22767286\ d10=-118.80939259\ d11=125.70367719\ d12=-115.32802387\ d13=-67.18444237\ d14=102.94732701\ d15=172.38788628\ d16=167.1055241\ d17=118.09484964\ d18=-23.44166578\ d19=35.24576457\ d20=-128.79801474\ d21=117.76006928\ d22=-121.26594429\ d23=121.73676873\ d24=-117.45422198\ d25=119.65551639\ d26=-121.99083617\ \Version=EM64L-G03RevE.01\HF=-614.6316009\ S2=0.755899\ S2-1=0.\ S2A=0.750019\ RMSD=9.072e-09\ RMSF=4.077e-05\ Thermal=0.\ Dipole=0.5831498,0.3307191,0.996724\ PG=C01 [X(C8H15O4)]\ \@

MPW1K/cc-pVDZ

1\1\GINC-I7\FTS\UmPW1PW91\CC-pVDZ\C8H15O4(2)\SUZUKI\20-May-2011\1\1\#mPW1PW91/cc-pVDZ IOp(3/76=0572004280) OPT=(TS,NoEigenTest,z-matrix,readFC,Maxcycle=100) Nosymm geom=check guess=read\THF TS MPW1K/cc-pVDZ\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,O\O,4,r4,3,a4,2,d4,O\H,1,r5,2,a5,5,d5,O\H,1,r6,2,a6,5,d6,O\H,2,r7,3,a7,1,d7,O\H,2,r8,3,a8,1,d8,O\H,3,r9,4,a9,2,d9,O\H,3,r10,4,a10,2,d10,O\H,4,r11,5,a11,3,d11,O\O,4,r12,5,a12,3,d12,O\O,13,r13,4,a13,5,d13,O\X,14,1,13,90,4,0,0\H,14,r14,15,a14,13,d14,O\X,16,1,14,90,15,0,0\C,16,r15,17,a15,14,d15,O\C,18,r16,16,a16,17,d16,O\C,19,r17,18,a17,16,d17,O\C,20,r18,19,a18,18,d18,O\O,21,r19,20,a19,19,d19,O\H,18,r20,19,a20,22,d20,O\H,19,r21,20,a21,18,d21,O\H,19,r22,20,a22,18,d22,O\H,20,r23,21,a23,19,d23,O\H,20,r24,21,a24,19,d24,O\H,21,r25,22,a25,20,d25,O\H,21,r26,22,a26,20,d26,O\|r1=1.51678988\r2=1.52625171\r3=1.52857024\r4=1.38316527\r5=1.09178562\r6=1.09896662\r7=1.09465167\r8=1.09297341\r9=1.0915203\r10=1.09370116\r11=1.09206184\r12=1.4114048\r13=1.3667547\r14=1.21883029\r15=1.30039503\r16=1.517843\r17=1.52756324\r18=1.51477421\r19=1.418723\r20=1.09263989\r21=1.09510579\r22=1.09340027\r23=1.09250292\r24=1.09482812\r25=1.09678217\r26=1.09180014\|a2=101.70564079\|a3=103.55394952\|a4=107.32841585\|a5=114.47021122\|a6=111.32389258\|a7=110.70368393\|a8=113.27120731\|a9=111.65399958\|a10=108.48440298\|a11=107.81015336\|a12=112.11363923\|a13=109.60388878\|a14=92.3317102\|a15=93.94272986\|a16=106.60918486\|a17=102.63267548\|a18=101.94280284\|a19=104.25968846\|a20=119.12320681\|a21=111.26940872\|a22=113.03410156\|a23=112.84394282\|a24=109.87292752\|a25=109.31588341\|a26=107.56720734\|d3=-20.444054\|d4=-2.41859948\|d5=117.44734847\|d6=-118.82835803\|d7=116.51308735\|d8=-121.84770939\|d9=122.33424382\|d10=-118.8330322\|d11=125.47900767\|d12=-115.46591708\|d13=-66.79306853\|d14=102.95745234\|d15=170.54983823\|d16=166.27235906\|d17=119.01500401\|d18=-24.03825573\|d19=36.2257846\|d20=-128.63008989\|d21=117.75604584\|d22=-121.14287025\|d23=121.9172129\|d24=-117.20464588\|d25=119.51473493\|d26=-121.9699836\|Version=EM64L-G03RevE.01\HF=-614.4561597\|S2=0.762286\|S2-1=0.\|S2A=0.750065\|RMSD=6.327e-09\|RMSF=2.503e-05\|Thermal=0.\|Dipole=0.5811044,0.3211749,0.974439\|PG=C01[X(C8H15O4)]\|@

MPWKIS1K/cc-pVDZ

1\1\GINC-I7\FTS\UmPWKCIS\CC-pVDZ\C8H15O4(2)\SUZUKI\20-May-2011\1\1\#MPWKIS/cc-pVDZ IOp(3/76=0590004100) OPT=(TS,NoEigenTest,z-matrix,readFC,Maxcycle=100) Nosymm geom=check guess=read\THF TS MPWKIS1K/cc-pVDZ\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,O\O,4,r4,3,a4,2,d4,O\H,1,r5,2,a5,5,d5,O\H,1,r6,2,a6,5,d6,O\H,2,r7,3,a7,1,d7,O\H,2,r8,3,a8,1,d8,O\H,3,r9,4,a9,2,d9,O\H,3,r10,4,a10,2,d10,O\H,4,r11,5,a11,3,d11,O\O,4,r12,5,a12,3,d12,O\O,13,r13,4,a13,5,d13,O\X,14,1,13,90,4,0,0\H,14,r14,15,a14,13,d14,O\X,16,1,14,90,15,0,0\C,16,r15,17,a15,14,d15,O\C,18,r16,16,a16,17,d16,O\C,19,r17,18,a17,16,d17,O\C,20,r18,19,a18,18,d18,O\O,21,r19,20,a19,19,d19,O\H,18,r20,19,a20,22,d20,O\H,19,r21,20,a21,18,d21,O\H,19,r22,20,a22,18,d22,O\H,20,r23,21,a23,19,d23,O\H,20,r24,21,a24,19,d24,O\H,21,r25,22,a25,20,d25,O\H,21,r26,22,a26,20,d26,O\|r1=1.51673657\r2=1.52563926\r3=1.52883018\r4=1.38525314\r5=1.09257293\r6=1.09978733\r7=1.09503885\r8=1.09328474\r9=1.09181576\r10=1.09409196\r11=1.09310323\r12=1.41354136\r13=1.36727539\r14=1.21975435\r15=1.30105774\r16=1.51727119\r17=1.52741636\r18=1.51488852\r19=1.41975622\r20=1.09362609\r21=1.09561613\r22=1.0937481\r23=1.09281589\r24=1.09518534\r25=1.09755655\r26=1.09256149\|a2=101.71746344\|a3=103.64542382\|a4=107.3515395\|a5=114.43871302\|a6=111.3051869\|a7=110.75079576\|a8=113.31907472\|a9=111.69751447\|a10=108.45801986\|a11=107.69428703\|a12=112.27903109\|a13=109.81460401\|a14=93.00738056\|a15=94.07545144\|a16=106.69501915\|a17=102.71363699\|a18=101.9929058\|a19=104.41290083\|a20=119.09793234\|a21=111.29081217\|a22=113.07454135\|a23=112.82178344\|a24=109.92607868\|a25=109.39475817\|a26=107.61421717\|d3=-20.85810039\|d4=-1.56695275\|d5=117.56907195\|d6=-119.03434082\|d7=116.6035855\|d8=-121.87107034\|d9=122.51172882\|d10=-118.83615091\|d11=125.27686614\|d12=-115.76145107\|d13=-67.27429549\|d14=103.33078043\|d15=171.24296222\|d16=166.59845637\|d17=119.6544918\|d18=-24.00740423\|d19=35.82293475\|d20=-128.61160678\|d21=117.79754305\|d22=-121.28188101\|d23=121.98922016\|d24=-117.30484554\|d25=119.6264359\|d26=-122.05626022\|Version=EM64L-G03RevE.01\HF=-614.2314966\|S2=0.759995\|S2-1=0.\|S2A=0.750046\|RMSD=5.692e-09\|RMSF=2.485e-05\|Thermal=0.\|Dipole=0.5730497,0.3163182,0.9823941\|PG=C01 [X(C8H15O4)]\|@

M05/cc-pVDZ

1\1\GINC-I7\FTS\UM05\CC-pVDZ\C8H15O4(2)\SUZUKI\20-May-2011\1\1\#M05/cc-pVDZ OPT=(TS,NoEigenTest,z-matrix,readFC,Maxcycle=100) Nosymm geom=check guess=read\THF TS M05/cc-pVDZ\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,O\O,4,r4,3,a4,2,d4,O\H,1,r5,2,a5,5,d5,O\H,1,r6,2,a6,5,d6,O\H,2,r7,3,a7,1,d7,O\H,2,r8,3,a8,1,d8,O\H,3,r9,4,a9,2,d9,O\H,3,r10,4,a10,2,d10,O\H,4,r11,5,a11,3,d11,O\O,4,r12,5,a12,3,d12,O\O,13,r13,4,a13,5,d13,O\X,14,1,13,90,4,0,0\H,14,r14,15,a14,13,d14,O\X,16,1,14,90,15,0,0\C,16,r15,17,a15,14,d15,O\C,18,r16,16,a16,17,d16,O\C,19,r17,18,a17,16,d17,O\C,20,r18,19,a18,18,d18,O\O,21,r19,20,a19,19,d19,O\H,18,r20,19,a20,22,d20,O\H,19,r21,20,a21,18,d21,O\H,19,r22,20,a22,18,d22,O\H,20,r23,21,a23,19,d23,O\H,20,r24,21,a24,19,d24,O\

H,21,r25,22,a25,20,d25,0\H,21,r26,22,a26,20,d26,0\|r1=1.51991474\r2=1.52825986\r3=1.53116133\r4=1.38924256\r5=1.0974071\r6=1.10533163\r7=1.09916803\r8=1.09739895\r9=1.09630393\r10=1.09846232\r11=1.09785328\r12=1.43233663\r13=1.3649374\r14=1.22511263\r15=1.31360876\r16=1.51944533\r17=1.53022784\r18=1.51741494\r19=1.42774359\r20=1.09871337\r21=1.10019836\r22=1.09799522\r23=1.09690372\r24=1.09953226\r25=1.10252985\r26=1.09734188\|a2=101.63469593\|a3=103.65028872\|a4=107.53067253\|a5=114.450522\|a6=111.30557798\|a7=110.75662606\|a8=113.25876981\|a9=111.66822098\|a10=108.55597147\|a11=107.82181448\|a12=112.37312053\|a13=110.48129862\|a14=92.05268776\|a15=95.09754874\|a16=106.31359414\|a17=102.81389724\|a18=102.04945312\|a19=104.47324349\|a20=119.38838331\|a21=111.1651591\|a22=113.08058037\|a23=112.69630057\|a24=109.94695494\|a25=109.18230136\|a26=107.40648013\|d3=-21.83655896\|d4=-0.1619484\|d5=117.47003713\|d6=-119.07067299\|d7=116.605362\|d8=-121.72903096\|d9=122.636749\|d10=-118.58385393\|d11=125.87227259\|d12=-115.72991993\|d13=-68.89872298\|d14=103.7629886\|d15=169.76691248\|d16=168.63241753\|d17=119.14404023\|d18=-24.5197289\|d19=35.82335783\|d20=-128.6891747\|d21=117.60672182\|d22=-121.38594648\|d23=121.88986232\|d24=-117.30145988\|d25=119.64333441\|d26=-122.08116708\|Version=EM64L-G03 RevE.01\HF=-614.2360272\|S2=0.755386\|S2-1=0.\|S2A=0.750019\|RMSD=2.071e-09\|RMSF=3.318e-05\|Thermal=0.\|Dipole=0.5253668,0.3108195,1.0497897\|PG=C01[X(C8H15O4)]\|@

G3(MP2)-RAD//MP2/cc-pVDZ

G3=-614.0020947

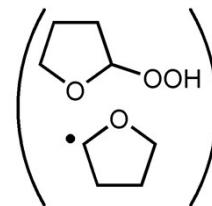
G3(MP2)-RAD//B3LYP/6-31G*

G3=-614.002426

Complex of 2-hydroperoxytetrahydrofuran and tetrahydrofuran-2-yl radical (7a)

HF/6-311G**

1\1\GINC-I7\FOpt\UHF\6-311G(d,p)\C8H15O4(2)\SUZUKI\27-May-2011\1\#HF/6-311G** OPT=(z-matrix,CalcFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THFooh-THFrAdical c
 complex HF/6-311G**\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\H,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\O,14,r14,13,a14,4,d14,0\C,15,r15,14,a15,13,d15,0\C,16,r16,15,a16,14,d16,0\C,17,r17,16,a17,15,d17,0\C,18,r18,17,a18,16,d18,0\O,19,r19,18,a19,17,d19,0\H,16,r20,15,a20,17,d20,0\H,17,r21,16,a21,18,d21,0\H,17,r22,16,a22,18,d22,0\H,18,r23,17,a23,19,d23,0\H,18,r24,17,a24,19,d24,0\H,19,r25,18,a25,20,d25,0\H,19,r26,18,a26,20,d26,0\|r1=1.52487518\r2=1.53739625\r3=1.50827435\r4=1.36338676\r5=1.08184922\r6=1.08410412\r7=1.08620028\r8=1.08254042\r9=1.0852218\r10=1.08667331\r11=1.0751755\r12=5.80151682\r13=0.94297327\r14=1.38295417\r15=1.40162632\r16=1.52093472\r17=1.53060179\r18=1.53113729\r19=1.42145793\r20=1.08122535\r21=1.08170649\r22=1.08542354\r23=1.08374179\r24=1.08321898\r25=1.08486583\r26=1.08059957\|a2=101.85339401\|a3=101.90200335\|a4=110.64739077\|a5=114.06084629\|a6=110.91161618\|a7=110.32150337\|a8=113.43473117\|a9=112.70100922\|a10=110.58033804\|a11=113.93428712\|a12=75.11845033\|a13=14.89714464\|a14=102.38927337\|a15=109.05976031\|a16=106.44134994\|a17=101.41619509\|a18=102.0597474\|a19=106.10115277\|a20=108.3768749\|a21=112.40394919\|a22=108.66092119\|a23=110.12892461\|a24=113.25515455\|a25=111.79798949\|a26=113.24599013\|d3=-26.49309626\|d4=10.8704484\|d5=117.76650925\|d6=-118.44388953\|d7=116.81864833\|d8=-120.8708131\|d9=121.49615261\|d10=-117.58055463\|d11=146.40536404\|d12=-40.9144918\|d13=-90.12734408\|d14=153.28390273\|d15=117.77747534\|d16=-176.363313\|d17=-85.51236496\|d18=-33.17043133\|d19=22.40309837\|d20=124.90103775\|d21=122.52827915\|d22=-116.9615321\|d23=117.56053213\|d24=-121.01038287\|d25=-117.17659618\|d26=119.77228494\|Version=EM64L-G03 RevE.01\HF=-611.1183341\|S2=0.76133\|S2-1=0.\|S2A=0.750094\|RMSD=5.543e-09\|RMSF=1.128e-06\|Thermal=0.\|Dipole=-0.1685135,1.1906796,-0.0124024\|PG=C01 [X(C8H15O4)]\|@



MP2/6-311G**

1\1\GINC-I7\FOpt\UMP2-FC\6-311G(d,p)\C8H15O4(2)\SUZUKI\31-May-2011\1\#MP2/6-311G** OPT=(z-matrix,readFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THFooh-THFrAdical complex MP2/6-311G**\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\H,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\O,14,r14,13,a14,4,d14,0\C,15,r15,14,a15,13,d15,0\C,16,r16,15,a16,14,d16,0\C,17,r17,16,a17,15,d17,0\C,18,r18,17,a18,16,d18,0\O,19,r19,18,a19,17,d19,0\H,16,r20,15,a20,17,d20,0\H,17,r21,16,a21,18,d21,0\H,17,r22,16,a22,18,d22,0\H,18,r23,17,a23,19,d23,0\H,18,r24,17,a24,19,d24,0\H,19,r25,18,a2

5,20,d25,0\H,19,r26,18,a26,20,d26,0\|r1=1.5236698\r2=1.53918513\r3=1.50498191\r4=1.37778388\r5=1.09149391\r6=1.09408322\r7=1.0947262\r8=1.09085649\r9=1.09411179\r10=1.09649096\r11=1.08412214\r12=5.46356226\r13=0.96509465\r14=1.45288565\r15=1.42174214\r16=1.52331981\r17=1.53166194\r18=1.53031041\r19=1.44716292\r20=1.09318728\r21=1.09119657\r22=1.09430843\r23=1.09269693\r24=1.09237034\r25=1.09573442\r26=1.09030045\|a2=100.7335561\|a3=101.56203962\|a4=111.08406644\|a5=114.75459386\|a6=110.29038641\|a7=110.36730376\|a8=113.38553511\|a9=112.79663724\|a10=110.63390393\|a11=113.29336094\|a12=81.18058074\|a13=10.48156357\|a14=98.69166551\|a15=106.63503976\|a16=104.69614391\|a17=100.66177061\|a18=101.62234826\|a19=106.20181292\|a20=108.548617\|a21=112.40820691\|a22=108.41710536\|a23=109.92881966\|a24=113.26914188\|a25=111.33343721\|a26=113.55428399\|d3=-31.25980567\|d4=14.38441269\|d5=116.96019746\|d6=-117.91961952\|d7=116.07508545\|d8=-119.98099267\|d9=121.69666834\|d10=-116.24008495\|d11=147.1873644\|d12=-34.65291313\|d13=-91.35085089\|d14=140.81862901\|d15=117.25631358\|d16=-176.87589607\|d17=-83.35393081\|d18=-36.89103767\|d19=26.54215569\|d20=125.11083589\|d21=122.40992626\|d22=-116.37869375\|d23=117.21544008\|d24=-120.54439844\|d25=-116.67238017\|d26=119.40746914\|Version=EM64L-G03RevE.01\HF=-611.1090741\MP2=-613.0642215\PUHF=-611.1121418\|PMP2-0=-613.0661386\|S2=0.761571\|S2-1=0.752847\|S2A=0.750099\|RMSD=7.857e-09\|RMSF=4.517e-06\|Thermal=0\|Dipole=-0.2709665,1.1823189,-0.0886285\|PG=C01 [X(C8H15O4)]\|@

MP2/cc-pVDZ

1\|GINC-I7\FOpt\UMP2-FC\CC-pVDZ\C8H15O4(2)\SUZUKI\02-Jun-2011\1\|MP2/cc-pVDZ OPT=(z-matrix,readFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THFohh-THFradiacal complex MP2/cc-pVDZ\|0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\H,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\O,14,r14,13,a14,4,d14,0\C,15,r15,14,a15,13,d15,0\C,16,r16,15,a16,14,d16,0\C,17,r17,16,a17,15,d17,0\C,18,r18,17,a18,16,d18,0\O,19,r19,18,a19,17,d19,0\H,16,r20,15,a20,17,d20,0\H,17,r21,16,a21,18,d21,0\H,17,r22,16,a22,18,d22,0\H,18,r23,17,a23,19,d23,0\H,18,r24,17,a24,19,d24,0\H,19,r25,18,a25,20,d25,0\H,19,r26,18,a26,20,d26,0\|r1=1.52771597\r2=1.54239936\r3=1.5084173\r4=1.38286965\r5=1.10059048\r6=1.10345771\r7=1.10378412\r8=1.0993799\r9=1.10256829\r10=1.10519962\r11=1.09370379\r12=5.39518929\r13=0.97319172\r14=1.46359822\r15=1.42515644\r16=1.52768442\r17=1.53484553\r18=1.53327579\r19=1.44980064\r20=1.1025361\r21=1.09988829\r22=1.10298366\r23=1.10183889\r24=1.10098573\r25=1.10534301\r26=1.09931236\|a2=100.74348662\|a3=101.59814825\|a4=111.12913519\|a5=114.74969894\|a6=110.2524215\|a7=110.48218942\|a8=113.42727832\|a9=112.97694997\|a10=110.44953626\|a11=113.3741602\|a12=82.48544596\|a13=10.74328638\|a14=98.06912248\|a15=106.06627081\|a16=104.72345765\|a17=100.69013076\|a18=101.62681748\|a19=106.22275444\|a20=108.48285397\|a21=112.42466637\|a22=108.53144071\|a23=109.86183169\|a24=113.46758785\|a25=111.34409569\|a26=113.63656183\|d3=-31.29109926\|d4=14.83050903\|d5=117.16252396\|d6=-118.13019554\|d7=116.27974435\|d8=-119.8956259\|d9=121.99875108\|d10=-116.03811697\|d11=147.92441971\|d12=-34.45393245\|d13=-86.51625699\|d14=144.47783209\|d15=118.62331796\|d16=-177.16399599\|d17=-83.84098829\|d18=-36.90301952\|d19=26.87455764\|d20=124.99612095\|d21=122.489219\|d22=-116.57771734\|d23=117.25012671\|d24=-120.86408678\|d25=-116.87696897\|d26=119.57758021\|Version=EM64L-G03RevE.01\HF=-610.9962195\MP2=-612.8413688\PUHF=-610.9992857\|PMP2-0=-612.8432803\|S2=0.761516\|S2-1=0.752798\|S2A=0.750098\|RMSD=3.777e-09\|RMSF=4.620e-07\|Thermal=0\|Dipole=-0.2558945,1.1644157,-0.0695861\|PG=C01 [X(C8H15O4)]\|@

MP2/aug-cc-pVDZ//MP2/cc-pVDZ

MP2=-612.979137

QCISD/6-311G**//MP2/cc-pVDZ

QCISD=-613.1634354

CCSD(T)/6-311G**//MP2/cc-pVDZ

CCSD(T)=-613.2338216

QCISD/cc-pVDZ//MP2/cc-pVDZ

QCISD=-612.9532529

CCSD(T)/cc-pVDZ//MP2/cc-pVDZ

CCSD(T)=-613.0106887

BHandHLYP/6-311G**

1\1\GINC-I7\FOpt\UBHandHLYP\6-311G(d,p)\C8H15O4(2)\SUZUKI\28-May-2011\1\1\#BHandHLYP/6-311G** OPT=(z-matrix, CalcFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THFooh-THFrAdical complex BHandHLYP/6-311G**\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\H,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\O,14,r14,13,a14,4,d14,0\C,15,r15,14,a15,13,d15,0\C,16,r16,15,a16,14,d16,0\C,17,r17,16,a17,15,d17,0\C,18,r18,17,a18,16,d18,0\O,19,r19,18,a19,17,d19,0\H,16,r20,15,a20,17,d20,0\H,17,r21,16,a21,18,d21,0\H,17,r22,16,a22,18,d22,0\H,18,r23,17,a23,19,d23,0\H,18,r24,17,a24,19,d24,0\H,19,r25,18,a25,20,d25,0\H,19,r26,18,a26,20,d26,0\|r1=1.5195675\r2=1.53439653\r3=1.49463163\r4=1.36286963\r5=1.08291486\r6=1.08533946\r7=1.08639937\r8=1.08239631\r9=1.08605626\r10=1.08892777\r11=1.07468717\r12=5.62525887\r13=0.95419597\r14=1.41340123\r15=1.41027238\r16=1.5177825\r17=1.526183\r18=1.52515914\r19=1.43116584\r20=1.08377327\r21=1.08224709\r22=1.08562345\r23=1.0842708\r24=1.08347335\r25=1.08634382\r26=1.08207517\|a2=101.84272297\|a3=101.92734386\|a4=111.26286963\|a5=114.32975277\|a6=110.8296494\|a7=110.36581639\|a8=113.26588222\|a9=112.92422518\|a10=110.8626798\|a11=114.36409685\|a12=75.76542039\|a13=12.41719521\|a14=101.07929885\|a15=108.14187247\|a16=105.83274174\|a17=101.51916333\|a18=102.26347448\|a19=106.11375384\|a20=108.19760693\|a21=112.26599006\|a22=108.62156722\|a23=110.02632408\|a24=113.14049367\|a25=111.86156927\|a26=113.43835443\|d3=-27.72179236\|d4=13.46550997\|d5=117.62237844\|d6=-118.17561857\|d7=117.08857914\|d8=-120.18993912\|d9=121.61740618\|d10=-117.1109588\|d11=151.51120079\|d12=-35.05747815\|d13=-96.40346519\|d14=142.42864011\|d15=119.0689695\|d16=-175.82703639\|d17=-85.91834586\|d18=-33.55884888\|d19=23.25422812\|d20=124.90796418\|d21=122.4568621\|d22=-117.16556863\|d23=117.62880057\|d24=-121.08297803\|d25=-117.02662624\|d26=119.55789734\|Version=EM64L-G03RevE.01\HF=-614.4146064\|S2=0.755612\|S2-1=0.\|S2A=0.750022\|RMSD=5.882e-09\|RMSF=1.051e-05\|Thermal=0.\|Dipole=-0.2434227,1.201711,-0.0616924\|PG=C01 [X(C8H15O4)]\|@

BHandHLYP/cc-pVDZ

1\1\GINC-I7\FOpt\UBHandHLYP\CC-pVDZ\C8H15O4(2)\SUZUKI\01-Jun-2011\1\1\#BHandHLYP/cc-pVDZ OPT=(z-matrix,read FC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THFooh-THFrAdical complex BHandHLYP/cc-pVDZ\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\H,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\O,14,r14,13,a14,4,d14,0\C,15,r15,14,a15,13,d15,0\C,16,r16,15,a16,14,d16,0\C,17,r17,16,a17,15,d17,0\C,18,r18,17,a18,16,d18,0\O,19,r19,18,a19,17,d19,0\H,16,r20,15,a20,17,d20,0\H,17,r21,16,a21,18,d21,0\H,17,r22,16,a22,18,d22,0\H,18,r23,17,a23,19,d23,0\H,18,r24,17,a24,19,d24,0\H,19,r25,18,a25,20,d25,0\H,19,r26,18,a26,20,d26,0\|r1=1.52023989\r2=1.53391243\r3=1.49533521\r4=1.36576061\r5=1.09136861\r6=1.0939935\r7=1.09451241\r8=1.09006143\r9=1.09372275\r10=1.09690345\r11=1.08355713\r12=5.48609555\r13=0.96059911\r14=1.41570182\r15=1.41079973\r16=1.51827962\r17=1.52595783\r18=1.52453452\r19=1.43031431\r20=1.09225798\r21=1.09021313\r22=1.09338786\r23=1.09251532\r24=1.0913829\r25=1.09531095\r26=1.09023139\|a2=101.76625036\|a3=101.86865987\|a4=111.23557149\|a5=114.31796971\|a6=110.77012757\|a7=110.42586491\|a8=113.2880921\|a9=113.0177344\|a10=110.65425475\|a11=114.27500015\|a12=79.51985589\|a13=12.55077757\|a14=100.78005235\|a15=107.73036208\|a16=105.9620384\|a17=101.49192246\|a18=102.14978806\|a19=106.10119297\|a20=108.14112604\|a21=112.18494662\|a22=108.64846055\|a23=109.97084958\|a24=113.31637084\|a25=111.77631158\|a26=113.46209955\|d3=-28.28701916\|d4=14.4948661\|d5=117.77216996\|d6=-118.27055452\|d7=117.04723978\|d8=-120.12754159\|d9=121.85842248\|d10=-116.81493567\|d11=151.59077996\|d12=-34.57980306\|d13=-86.21074028\|d14=148.12448201\|d15=118.65777081\|d16=-175.94085294\|d17=-86.37060601\|d18=-34.03823688\|d19=24.4747401\|d20=124.86600936\|d21=122.55654232\|d22=-117.1904978\|d23=117.49174704\|d24=-121.26409754\|d25=-117.19310415\|d26=119.58920701\|Version=EM64L-G03RevE.01\HF=-614.2892514\|S2=0.755513\|S2-1=0.\|S2A=0.750022\|RMSD=5.531e-09\|RMSF=1.210e-05\|Thermal=0.\|Dipole=-0.237007,1.1791397,-0.0505318\|PG=C01 [X(C8H15O4)]\|@

BHandHLYP/aug-cc-pVDZ//BHandHLYP/cc-pVDZ

HF=-614.3343956

B3LYP/6-311G**

1\1\GINC-I7\FOpt\UB3LYP\6-311G(d,p)\C8H15O4(2)\SUZUKI\27-May-2011\1\1\#B3LYP/6-311G** OPT=(z-matrix,CalcFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THFooh-THFrAdical complex B3LYP/6-311G**\0,2\C\C,1,r1\C,2,r2,1,a2\C,3,r3,2,a3,1,d3,0\O,4,r4,3,a4,2,d4,0\H,1,r5,2,a5,5,d5,0\H,1,r6,2,a6,5,d6,0\H,2,r7,3,a7,1,d7,0\H,2,r8,3,a8,1,d8,0\H,3,r9,4,a9,2,d9,0\H,3,r10,4,a10,2,d10,0\H,4,r11,5,a11,3,d11,0\H,4,r12,5,a12,3,d12,0\O,13,r13,4,a13,5,d13,0\O,14,r14,13,a14,4,d14,0\C,15,r15,14,a15,13,d15,0\C,16,r16,15,a16,14,d16,0\C,17,r17,16,a17,15,d17,0\C,18,r18,17,a18,16,d18,0\O,19,r19,18,a19,17,d19,0\H,16,r20,15,a20,17,d20,0\H,17,r21,16,a21,18,d21,0\H,17,r22,16,a22,18,d22,0\H,18,r23,17,a23,19,d23,0\H,18,r24,17,a24,19,d24,0\H,19,r25,18,a

d14=147.69083395\d15=116.79951421\d16=-175.99973328\d17=-85.6239046\d18=-34.50879196\d19=24.54822157\d20=124.89230524\d21=122.56394402\d22=-117.16094931\d23=117.47386397\d24=-121.30635098\d25=-117.32441991\d26=119.82121483\\Version=EM64L-G03RevE.01\\HF=-614.4685406\\S2=0.755389\\S2-1=0.\\S2A=0.750021\\RMSD=7.071e-09\\RMSF=1.768e-05\\Thermal=0.\\Dipole=-0.2392965,1.1539674,-0.0652901\\PG=C01 [X(C8H15O4)]\\@

MPWK CIS1K/cc-pVDZ

1\\GINC-I7\\FOpt\\UmPWKCIS\\CC-pVDZ\\C8H15O4(2)\\SUZUKI\\06-Jun-2011\\1\\#MPWK CIS/cc-pVDZ IOp(3/76=0590004100) OPT=(z-matrix,readFC,Maxcycle=100)Nosymm geom=check guess=read\\THFooh-THFrAdical MPWK CIS/cc-pVDZ\\0,2\\C\\C,1,r1\\C,2,r2,1,a2\\C,3,r3,2,a3,1,d3,0\\O,4,r4,3,a4,2,d4,0\\H,1,r5,2,a5,5,d5,0\\H,1,r6,2,a6,5,d6,0\\H,2,r7,3,a7,1,d7,0\\H,2,r8,3,a8,1,d8,0\\H,3,r9,4,a9,2,d9,0\\H,3,r10,4,a10,2,d10,0\\H,4,r11,5,a11,3,d11,0\\H,4,r12,5,a12,3,d12,0\\O,13,r13,4,a13,5,d13,0\\O,14,r14,13,a14,4,d14,0\\C,15,r15,14,a15,13,d15,0\\C,16,r16,15,a16,14,d16,0\\C,17,r17,16,a17,15,d17,0\\C,18,r18,17,a18,16,d18,0\\O,19,r19,18,a19,17,d19,0\\H,16,r20,15,a20,17,d20,0\\H,17,r21,16,a21,18,d21,0\\H,17,r22,16,a22,18,d22,0\\H,18,r23,17,a23,19,d23,0\\H,18,r24,17,a24,19,d24,0\\H,19,r25,18,a25,20,d25,0\\H,19,r26,18,a26,20,d26,0\\r1=1.51589242\\r2=1.52873801\\r3=1.48969513\\r4=1.36279867\\r5=1.09335811\\r6=1.09711555\\r7=1.09591917\\r8=1.09178727\\r9=1.09539542\\r10=1.09935535\\r11=1.08497625\\r12=5.56986105\\r13=0.96212052\\r14=1.41076679\\r15=1.40900574\\r16=1.51492812\\r17=1.52067754\\r18=1.52051696\\r19=1.42575813\\r20=1.09565769\\r21=1.09175851\\r22=1.09474157\\r23=1.09408771\\r24=1.09279354\\r25=1.09755584\\r26=1.09322611\\a2=101.68920272\\a3=101.79850329\\a4=111.54622165\\a5=114.3853482\\a6=110.71881784\\a7=110.47625335\\a8=113.37627338\\a9=113.12586998\\a10=110.92246366\\a11=114.40957722\\a12=80.13612572\\a13=12.02017443\\a14=100.71638918\\a15=107.93249596\\a16=105.91393635\\a17=101.41593684\\a18=102.17585218\\a19=106.40723291\\a20=108.21567574\\a21=112.30137293\\a22=108.57072253\\a23=110.00053557\\a24=113.39788704\\a25=111.82205769\\a26=113.21235958\\d3=-28.11239999\\d4=14.01643728\\d5=118.09057714\\d6=-118.45347537\\d7=117.06464075\\d8=-120.27738584\\d9=121.92483121\\d10=-117.02057439\\d11=153.0857235\\d12=-35.41706027\\d13=-94.03493524\\d14=140.81274885\\d15=115.7151339\\d16=-175.6033508\\d17=-86.05051162\\d18=-33.84792126\\d19=23.56282699\\d20=124.74018974\\d21=122.66109857\\d22=-117.29521474\\d23=117.58935017\\d24=-121.41408199\\d25=-117.4626352\\d26=120.00840082\\Version=EM64L-G03RevE.01\\HF=-614.2436737\\S2=0.75463\\S2-1=0.\\S2A=0.750015\\RMSD=3.461e-09\\RMSF=1.772e-05\\Thermal=0.\\Dipole=-0.2579317,1.1560927,-0.057637\\PG=C01 [X(C8H15O4)]\\@

M05/cc-pVDZ

1\\GINC-I7\\FOpt\\UM05\\CC-pVDZ\\C8H15O4(2)\\SUZUKI\\07-Jun-2011\\1\\#M05/cc-pVDZ scf=qc OPT=(z-matrix,readFC,Maxcycle=100) NoSymm freq=NoRaman geom=check guess=read\\THFooh-THFrAdical M05/cc-pVDZ\\0,2\\C\\C,1,r1\\C,2,r2,1,a2\\C,3,r3,2,a3,1,d3,0\\O,4,r4,3,a4,2,d4,0\\H,1,r5,2,a5,5,d5,0\\H,1,r6,2,a6,5,d6,0\\H,2,r7,3,a7,1,d7,0\\H,2,r8,3,a8,1,d8,0\\H,3,r9,4,a9,2,d9,0\\H,3,r10,4,a10,2,d10,0\\H,4,r11,5,a11,3,d11,0\\H,4,r12,5,a12,3,d12,0\\O,13,r13,4,a13,5,d13,0\\O,14,r14,13,a14,4,d14,0\\C,15,r15,14,a15,13,d15,0\\C,16,r16,15,a16,14,d16,0\\C,17,r17,16,a17,15,d17,0\\C,18,r18,17,a18,16,d18,0\\O,19,r19,18,a19,17,d19,0\\H,16,r20,15,a20,17,d20,0\\H,17,r21,16,a21,18,d21,0\\H,17,r22,16,a22,18,d22,0\\H,18,r23,17,a23,19,d23,0\\H,18,r24,17,a24,19,d24,0\\H,19,r25,18,a25,20,d25,0\\H,19,r26,18,a26,20,d26,0\\r1=1.51922955\\r2=1.53254151\\r3=1.48799276\\r4=1.37045183\\r5=1.09842631\\r6=1.10228291\\r7=1.09988406\\r8=1.0958762\\r9=1.09975087\\r10=1.10494834\\r11=1.08936371\\r12=5.37628115\\r13=0.97068221\\r14=1.41204628\\r15=1.42540998\\r16=1.51857356\\r17=1.52347733\\r18=1.5223723\\r19=1.43208435\\r20=1.10155036\\r21=1.09590934\\r22=1.09878771\\r23=1.09870051\\r24=1.09698845\\r25=1.10319038\\r26=1.09756363\\a2=101.726763\\a3=101.62859215\\a4=111.89655684\\a5=114.44311012\\a6=110.71352128\\a7=110.51154986\\a8=113.14656233\\a9=113.1390363\\a10=111.38430602\\a11=114.60060114\\a12=84.55962335\\a13=11.21243631\\a14=100.93379175\\a15=108.36829707\\a16=105.76420562\\a17=101.60462622\\a18=102.10790052\\a19=106.27350812\\a20=107.75595391\\a21=112.32563637\\a22=108.49539933\\a23=110.01955229\\a24=113.28676105\\a25=111.74086118\\a26=113.39229621\\d3=-28.88328274\\d4=15.58370673\\d5=118.02251578\\d6=-118.24693304\\d7=117.21541901\\d8=-119.90209216\\d9=121.69133752\\d10=-116.75498422\\d11=156.71097165\\d12=-35.05820924\\d13=-56.55695664\\d14=171.46645192\\d15=111.30905124\\d16=-175.97990993\\d17=-87.67153062\\d18=-34.0753141\\d19=25.21171842\\d20=124.48558353\\d21=122.76491259\\d22=-117.22089377\\d23=117.56949145\\d24=-121.3174558\\d25=-117.41396225\\d26=119.64620904\\Version=EM64L-G03RevE.01\\HF=-614.2479612\\S2=0.754564\\S2-1=0.\\S2A=0.750016\\RMSD=3.755e-09\\RMSF=3.461e-05\\Thermal=0.\\Dipole=-0.2021284,1.1649038,-0.0836779\\PG=C01 [X(C8H15O4)]\\@

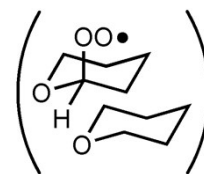
G3(MP2)-RAD//MP2/cc-pVDZ

G3=-614.0202439

G3(MP2)-RAD//B3LYP/6-31G*

G3=-614.0203949

Complex of THP and tetrapyrrole-2-peroxyl radical (5b)



HF/6-311G**

1\1\GINC-I7FOpt\UHF\6-311G(d,p)\C10H19O4(2)\SUZUKI\11-Oct-2011\1\#HF/6-311G** OPT=(z-matrix,CalcFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THP-THP radical complex HF/6-311G**\0,2\C\C,1,B1\C,1,B2,2,A1\C,2,B3,1,A2,3,D1,0\H,1,B4,3,A3,2,D2,0\H,2,B5,1,A4,3,D3,0\H,3,B6,1,A5,2,D4,0\H,4,B7,2,A6,1,D5,0\H,1,B8,3,A7,2,D6,0\H,2,B9,1,A8,3,D7,0\H,3,B10,1,A9,2,D8,0\H,4,B11,2,A10,1,D9,0\O,4,B12,2,A11,1,D10,0\H,3,B13,1,A12,13,D11,0\C,3,B14,1,A13,13,D12,0\C,15,B15,3,A14,1,D13,0\C,16,B16,15,A15,3,D14,0\C,17,B17,16,A16,15,D15,0\H,17,B18,16,A17,15,D16,0\H,18,B19,17,A18,16,D17,0\H,15,B20,3,A19,1,D18,0\H,17,B21,16,A20,15,D19,0\H,18,B22,17,A21,16,D20,0\C,15,B23,3,A22,1,D21,0\H,24,B24,15,A23,3,D22,0\H,24,B25,15,A24,3,D23,0\O,17,B26,16,A25,15,D24,0\C,13,B27,4,A26,2,D25,0\H,28,B28,13,A27,4,D26,0\H,28,B29,13,A28,4,D27,0\O,16,B30,15,A29,3,D28,0\O,31,B31,16,A30,15,D29,0\H,16,B32,15,A31,3,D30,0\B1=2.50700039\B2=1.53083754\B3=1.52394543\B4=1.08792966\B5=1.08792704\B6=1.08925474\B7=1.09027627\B8=1.08725984\B9=1.08725304\B10=1.08621708\B11=1.08284349\B12=1.40321025\B13=8.11604614\B14=7.20168832\B15=2.52103131\B16=2.37238547\B17=1.52025218\B18=1.08365684\B19=1.08798355\B20=1.0868787\B21=1.08085191\B22=1.08619603\B23=1.52955572\B24=1.08393545\B25=1.08723516\B26=1.42116023\B27=1.40313103\B28=1.08304232\B29=1.08996575\B30=1.44134813\B31=1.28802496\B32=1.07977747\A1=35.0319432\A2=86.99831544\A3=109.71066833\A4=94.47626572\A5=109.27335685\A6=110.32137538\A7=110.92244179\A8=145.55475508\A9=110.70639691\A10=111.02212523\A11=111.35026584\A12=52.38525572\A13=56.66725193\A14=64.01744138\A15=61.2681098\A16=92.39718003\A17=95.942853\A18=109.38703507\A19=38.27565151\A20=135.79189088\A21=109.14845783\A22=91.32156454\A23=111.82976816\A24=109.88228584\A25=30.85481175\A26=113.46314358\A27=106.46058984\A28=109.6352433\A29=96.40393311\A30=111.74178935\A31=145.5370214\D1=132.87398508\D2=-68.45369096\D3=-118.48818425\D4=-119.95527957\D5=-93.42524245\D6=173.00342932\D7=11.67835571\D8=122.61035852\D9=146.9517335\D10=28.4689413\D11=-36.16297898\D12=-35.00810261\D13=197.61154231\D14=-68.12120189\D15=-18.88761974\D16=92.28405162\D17=-90.80202014\D18=-20.14261289\D19=-143.53329425\D20=151.80766226\D21=218.84288131\D22=87.1666553\D23=206.32657925\D24=-148.78211297\D25=-60.4383526\D26=-178.28980725\D27=-61.6571438\D28=22.33551734\D29=103.2720708\D30=154.35365365\Version=EM64L-G03RevE.01\HF=-689.2362609\S2=0.760918\S2-1=0\S2A=0.750082\RMSD=9.041e-09\RMSF=7.351e-07\Thermal=0\Dipole=-0.3245919,0.2060009,-0.2890441\PG=C01 [X(C10H19O4)]\@

BHandHLYP/6-311G**

1\1\GINC-I7FOptUBHandHLYP\6-311G(d,p)\C10H19O4(2)\SUZUKI\12-Oct-2011\1\#BHandHLYP/6-311G** OPT=(z-matrix,readFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THP-THP radical complex BHandHLYP/6-311G**\0,2\C\C,1,B1\C,1,B2,2,A1\C,2,B3,1,A2,3,D1,0\H,1,B4,3,A3,2,D2,0\H,2,B5,1,A4,3,D3,0\H,3,B6,1,A5,2,D4,0\H,4,B7,2,A6,1,D5,0\H,1,B8,3,A7,2,D6,0\H,2,B9,1,A8,3,D7,0\H,3,B10,1,A9,2,D8,0\H,4,B11,2,A10,1,D9,0\O,4,B12,2,A11,1,D10,0\H,3,B13,1,A12,13,D11,0\C,3,B14,1,A13,13,D12,0\C,15,B15,3,A14,1,D13,0\C,16,B16,15,A15,3,D14,0\C,17,B17,16,A16,15,D15,0\H,17,B18,16,A17,15,D16,0\H,18,B19,17,A18,16,D17,0\H,15,B20,3,A19,1,D18,0\H,17,B21,16,A20,15,D19,0\H,18,B22,17,A21,16,D20,0\C,15,B23,3,A22,1,D21,0\H,24,B24,15,A23,3,D22,0\H,24,B25,15,A24,3,D23,0\O,17,B26,16,A25,15,D24,0\C,13,B27,4,A26,2,D25,0\H,28,B28,13,A27,4,D26,0\H,28,B29,13,A28,4,D27,0\O,16,B30,15,A29,3,D28,0\O,31,B31,16,A30,15,D29,0\H,16,B32,15,A31,3,D30,0\B1=2.49872988\B2=1.52523173\B3=1.51865976\B4=1.08840693\B5=1.08839288\B6=1.08971981\B7=1.09140805\B8=1.08747863\B9=1.08753584\B10=1.08650018\B11=1.08421227\B12=1.41036547\B13=8.04120164\B14=7.08947973\B15=2.51121743\B16=2.37094344\B17=1.51413074\B18=1.08610191\B19=1.08852064\B20=1.08751105\B21=1.08220155\B22=1.08656147\B23=1.52332276\B24=1.08402013\B25=1.08770848\B26=1.43149134\B27=1.41093422\B28=1.08425826\B29=1.0912136\B30=1.46623136\B31=1.29086659\B32=1.08214225\A1=35.00249962\A2=87.11885536\A3=109.71967306\A4=94.30618941\A5=109.20452827\A6=110.43138022\A7=110.99042473\A8=145.64964671\A9=110.76194655\A10=111.21238126\A11=111.39398631\A12=53.33038872\A13=57.15801919\A14=59.22430248\A15=61.14294824\A16=92.01489486\A17=95.93913786\A18=109.51197347\A19=42.18227903\A20=135.60876895\A21=109.06414285\A22=86.75728102\A23=112.14259725\A24=110.01379186\A25=31.11177337\A26=112.47135347\A27=106.21950352\A28=109.5615368\A29=96.10327419\A30=112.11962609\A31=146.10373936\D1=132.55607301\D2=-68.07292067\D3=-118.81239157\D4=-119.87828311\D5=-92.77874265\D6=173.35388919\D7=11.08293749\D8=122.75136993\D9=147.35646811\D10=28.97911138\D11=-31.48469779\D12=-30.23191651\D13=198.97107398\D14=-67.53342539\D15=-19.49330882\D16=91.86249182\D17=-89.9351486\D18=-15.33271182\D19=-143.80250582\D20=152.73252416\D21=220.34431617\D2

2=88.21883713\D23=207.84654589\D24=-150.16003872\D25=-60.75499071\D26=-177.9479469\D27=-61.37209306\D28=23.04949225\D29=97.87225527\D30=153.10994045\Version=EM64L-G03RevE.01\HF=-693.0376048\S2=0.756334\S2-1=0.\S2A=0.750023\RMSD=2.616e-09\RMSF=5.193e-06\Thermal=0.\Dipole=-0.4798368,0.1913313,-0.1010117\PG=C01 [X(C10H19O4)]\@

BHandHLYP/cc-pVDZ

1\1\GINC-I7\FOpt\UBHandHLYP\CC-pVDZ\C10H19O4(2)\SUZUKI\13-Oct-2011\1\1\#BHandHLYP/cc-pVDZ OPT=(z-matrix,readFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THP-THPooradical complex BHandHLYP/cc-pVDZ\0,2\C\C,1,B1\C,1,B2,2,A1\C,2,B3,1,A2,3,D1,0\H,1,B4,3,A3,2,D2,0\H,2,B5,1,A4,3,D3,0\H,3,B6,1,A5,2,D4,0\H,4,B7,2,A6,1,D5,0\H,1,B8,3,A7,2,D6,0\H,2,B9,1,A8,3,D7,0\H,3,B10,1,A9,2,D8,0\H,4,B11,2,A10,1,D9,0\O,4,B12,2,A11,1,D10,0\H,3,B13,1,A12,13,D11,0\C,3,B14,1,A13,13,D12,0\C,15,B15,3,A14,1,D13,0\C,16,B16,15,A15,3,D14,0\C,17,B17,16,A16,15,D15,0\H,17,B18,16,A17,15,D16,0\H,18,B19,17,A18,16,D17,0\H,15,B20,3,A19,1,D18,0\H,17,B21,16,A20,15,D19,0\H,18,B22,17,A21,16,D20,0\C,15,B23,3,A22,1,D21,0\H,24,B24,15,A23,3,D22,0\H,24,B25,15,A24,3,D23,0\O,17,B26,16,A25,15,D24,0\C,13,B27,4,A26,2,D25,0\H,28,B28,13,A27,4,D26,0\H,28,B29,13,A28,4,D27,0\O,16,B30,15,A29,3,D28,0\O,31,B31,16,A30,15,D29,0\H,16,B32,15,A31,3,D30,0\B1=2.49752898\B2=1.52503972\B3=1.51894454\B4=1.09647374\B5=1.09648572\B6=1.09785604\B7=1.09927184\B8=1.09522279\B9=1.09523929\B10=1.0944663\B11=1.09229054\B12=1.41057419\B13=7.87656882\B14=6.96165933\B15=2.51270938\B16=2.36772499\B17=1.51451054\B18=1.09435477\B19=1.09658947\B20=1.09584213\B21=1.09036181\B22=1.09437334\B23=1.52343124\B24=1.09159794\B25=1.09545535\B26=1.43121316\B27=1.41121213\B28=1.09252617\B29=1.09903597\B30=1.46625991\B31=1.29236113\B32=1.09059077\A1=35.02952377\A2=87.10516166\A3=109.69425968\A4=94.28163263\A5=109.20677234\A6=110.44640133\A7=111.06535689\A8=145.76053491\A9=110.84751207\A10=111.23885824\A11=111.40807741\A12=49.27049894\A13=53.69034813\A14=62.67052504\A15=61.14979561\A16=92.11299982\A17=95.62268814\A18=109.51481274\A19=37.5023397\A20=135.89634519\A21=109.14632977\A22=88.60130498\A23=112.19466621\A24=110.05779987\A25=31.31869232\A26=112.27007678\A27=106.19692852\A28=109.7409011\A29=96.31445748\A30=111.86975678\A31=145.9903515\B1=132.65862734\B2=-68.03906588\B3=-118.74510981\B4=-119.86551985\B5=-92.88920069\B6=173.47155941\B7=11.02205608\B8=122.87267166\B9=147.41534689\B10=29.0335213\B11=-31.88851609\B12=-30.10368316\B13=196.16786418\B14=-71.28173543\B15=-19.50151155\B16=91.67601065\B17=-89.85156083\B18=-15.16577881\B19=-144.16466015\B20=152.88650562\B21=219.26992436\B22=83.71934633\B23=203.37674009\B24=-149.67867008\B25=-60.87256578\B26=-177.73733083\B27=-61.24017342\B28=18.98119417\B29=96.18473948\B30=149.29960794\Version=EM64L-G03RevE.01\HF=-692.8974606\S2=0.755789\S2-1=0.\S2A=0.75002\RM SD=3.249e-09\RMSF=7.042e-06\Thermal=0.\Dipole=-0.4443752,0.1321851,-0.1955101\PG=C01 [X(C10H19O4)]\@

BHandHLYP/aug-cc-pVDZ//BHandHLYP/cc-pVDZ

HF=-692.9436736

MPW1K/cc-pVDZ

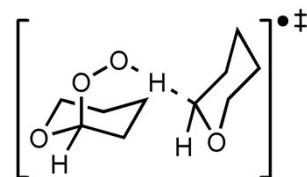
1\1\GINC-I7\FOpt\UmPW1PW91\CC-pVDZ\C10H19O4(2)\SUZUKI\13-Oct-2011\1\1\#mPW1PW91/cc-pVDZ IOp(3/76=0572004280) OPT=(z-matrix,readFC,Maxcycle=100) Nosymm geom=check guess=read\THP-THPooradical complex mPW1PW91/cc-pVDZ\0,2\C\C,1,B1\C,1,B2,2,A1\C,2,B3,1,A2,3,D1,0\H,1,B4,3,A3,2,D2,0\H,2,B5,1,A4,3,D3,0\H,3,B6,1,A5,2,D4,0\H,4,B7,2,A6,1,D5,0\H,1,B8,3,A7,2,D6,0\H,2,B9,1,A8,3,D7,0\H,3,B10,1,A9,2,D8,0\H,4,B11,2,A10,1,D9,0\O,4,B12,2,A11,1,D10,0\H,3,B13,1,A12,13,D11,0\C,3,B14,1,A13,13,D12,0\C,15,B15,3,A14,1,D13,0\C,16,B16,15,A15,3,D14,0\C,17,B17,16,A16,15,D15,0\H,17,B18,16,A17,15,D16,0\H,18,B19,17,A18,16,D17,0\H,15,B20,3,A19,1,D18,0\H,17,B21,16,A20,15,D19,0\H,18,B22,17,A21,16,D20,0\C,15,B23,3,A22,1,D21,0\H,24,B24,15,A23,3,D22,0\H,24,B25,15,A24,3,D23,0\O,17,B26,16,A25,15,D24,0\C,13,B27,4,A26,2,D25,0\H,28,B28,13,A27,4,D26,0\H,28,B29,13,A28,4,D27,0\O,16,B30,15,A29,3,D28,0\O,31,B31,16,A30,15,D29,0\H,16,B32,15,A31,3,D30,0\B1=2.48827381\B2=1.52020842\B3=1.5149025\B4=1.0976565\B5=1.09766469\B6=1.09915354\B7=1.10153501\B8=1.09617511\B9=1.09619689\B10=1.09562458\B11=1.0936726\B12=1.40609101\B13=7.89868532\B14=6.9837963\B15=2.50448713\B16=2.35437507\B17=1.51025615\B18=1.09686892\B19=1.09777716\B20=1.09719111\B21=1.09180043\B22=1.09535738\B23=1.51840211\B24=1.09313469\B25=1.09653242\B26=1.42583285\B27=1.4066583\B28=1.09384874\B29=1.1014123\B30=1.46355157\B31=1.28559912\B32=1.09292934\A1=35.073519\A2=87.0112828\A3=109.7535637\A4=94.28694267\A5=109.20421826\A6=110.34412037\A7=111.14843463\A8=145.89507329\A9=110.93457321\A10=111.23152332\A11=111.52743875\A12=49.47679396\A13=53.92279607\A14=63.20229278\A15=61.20851527\A16=92.17897633\A17=95.5174445\A18=109.50802951\A19=37.50888274\A20=136.23726658\A21=109.16258022\A22=89.40811817\A23=112.32818472\A24=110.20068366\A25=31.57878742\A26=111.81568262\A27=106.24563744\A28=109.78201317\A29=96.2579579\A30=111.91782259\A31=145.98629862\B1=132.62402559\B2=-67.99194621\B3=-118.81294374\B4=-119.8115438\B5=-92.70720472\B6=173.5253414\B7=10.96744127\B8=122.98044478\B9=147.82

44065\D10=29.30683884\D11=-32.49164434\D12=-30.80632432\D13=196.06568887\D14=-70.2871216\D15=-19.58809798\D16=91.573045\D17=-89.74599188\D18=-16.90541359\D19=-144.58953992\D20=153.07939257\D21=218.81533725\D22=84.02352634\D23=203.80030618\D24=-149.56282638\D25=-61.13784392\D26=-177.37191286\D27=-61.00109074\D28=19.80549373\D29=94.4591767\D30=149.93709291\\Version=EM64L-G03RevE.01\HF=-693.1149873\S2=0.754988\S2-1=0.\S2A=0.750015\RMSD=4.367e-09\RMSF=1.691e-05\Thermal=0.\Dipole=-0.4529403,0.1108363,-0.1753156\PG=C01 [X(C10H19O4)]\@

Most stable transition state involved in the abstraction of α -hydrogen in THP (6b)

HF/6-311G**

1\GINC-I7\FTS\UHF\6-311G(d,p)\C10H19O4(2)\SUZUKI\31-Dec-2011\I\#HF/6-311G** O
PT=(TS,NoEigenTest,z-matrix,readFC,Maxcycle=100) NoSymm geom=check guess=read\TH
P TS1 HF/6-311G**\0,2\H\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\O,4,B4,3,A3,2,D2,0\O,4,B5,3,A4,2,D3,0\O,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,6,B8,4,A7,3,D6,0\H,7,B9,3,A8,2,D7,0\H,2,B10,1,A9,6,D8,0\H,3,B11,2,A10,1,D9,0\H,6,B12,4,A11,3,D10,0\H,7,B13,3,A12,2,D11,0\H,4,B14,3,A13,2,D12,0\H,4,B15,3,A14,2,D13,0\O,4,B16,3,A15,2,D14,0\O,17,B17,4,A16,3,D15,0\H,18,B18,17,A17,4,D16,0\O,18,B19,17,A18,4,D17,0\O,20,B20,18,A19,17,D18,0\O,21,B21,20,A20,18,D19,0\O,21,B22,20,A21,18,D20,0\O,20,B23,18,A22,17,D21,0\O,20,B24,18,A23,17,D22,0\H,21,B25,20,A24,18,D23,0\H,22,B26,21,A25,20,D24,0\H,23,B27,21,A26,20,D25,0\H,24,B28,20,A27,18,D26,0\H,21,B29,20,A28,18,D27,0\H,22,B30,21,A29,20,D28,0\H,23,B31,21,A30,20,D29,0\H,24,B32,20,A31,18,D30,0\B1=1.08534574\B2=2.50096702\B3=2.35385355\B4=1.36831538\B5=1.5152058\B6=1.52130955\B7=1.08820919\B8=1.09012865\B9=1.08777987\B10=1.08754313\B11=1.08116847\B12=1.08477803\B13=1.08652446\B14=1.08025969\B15=1.31901816\B16=2.53410073\B17=1.3561831\B18=2.0233218\B19=1.41977176\B20=2.37002246\B21=2.49653315\B22=1.52101331\B23=1.52325062\B24=1.37458071\B25=1.08621172\B26=1.08702475\B27=1.08791739\B28=1.08771339\B29=1.0814396\B30=1.0856149\B31=1.08691275\B32=1.08338952\A1=145.46095188\A2=62.15714018\A3=32.76105877\A4=93.39276593\A5=35.05555981\A6=93.67501731\A7=107.97076475\A8=109.0703185\A9=107.07722287\A10=146.30006355\A11=109.23838235\A12=109.20101092\A13=141.68459369\A14=93.67211523\A15=93.77232659\A16=107.29588088\A17=86.04365588\A18=109.70446291\A19=93.23258672\A20=62.40600084\A21=92.84785223\A22=111.85915935\A23=106.80634979\A24=94.85006528\A25=93.72883821\A26=109.07972812\A27=107.08651721\A28=136.72131378\A29=145.62408427\A30=109.47972734\A31=109.79600795\B1=138.07208243\B2=-149.36259954\B3=-14.91573466\B4=-7.44674236\B5=-128.36797948\B6=-96.76121787\B7=120.70935386\B8=118.95110827\B9=3.22088374\B10=146.67852733\B11=-122.14241379\B12=-153.7575963\B13=90.84044693\B14=88.96910404\B15=139.26914889\B16=-125.37660423\B17=-105.57727567\B18=174.52447693\B19=-96.36257788\B20=-114.65197914\B21=80.91213328\B22=-155.70917706\B23=-3.65095652\B24=93.95254686\B25=-91.55889771\B26=-170.54263275\B27=119.42772437\B28=-138.22649023\B29=151.11898723\B30=-54.34900065\\Version=EM64L-G03RevE.01\HF=-689.1724144\S2=0.796972\S2-1=0.\S2A=0.750767\RMSD=6.454e-09\RMSF=3.330e-05\Thermal=0.\Dipole=0.8871277,0.543591,-0.3835816\PG=C01 [X(C10H19O4)]\@



BHandHLYP/6-311G**

1\GINC-I7\FTS\UBHandHLYP\6-311G(d,p)\C10H19O4(2)\SUZUKI\20-Jul-2011\I\#BHandHLYP/6-311G** OPT=(TS,NoEigenTest,z-matrix,readFC,Maxcycle=100) NoSymm geom=check guess=read\THP TS1 BHandHLYP/6-311G**\0,2\H\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\O,4,B4,3,A3,2,D2,0\O,4,B5,3,A4,2,D3,0\O,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,6,B8,4,A7,3,D6,0\H,7,B9,3,A8,2,D7,0\H,2,B10,1,A9,6,D8,0\H,3,B11,2,A10,1,D9,0\H,6,B12,4,A11,3,D10,0\H,7,B13,3,A12,2,D11,0\H,4,B14,3,A13,2,D12,0\H,4,B15,3,A14,2,D13,0\O,4,B16,3,A15,2,D14,0\O,17,B17,4,A16,3,D15,0\H,18,B18,17,A17,4,D16,0\O,18,B19,17,A18,4,D17,0\O,20,B20,18,A19,17,D18,0\O,21,B21,20,A20,18,D19,0\O,21,B22,20,A21,18,D20,0\O,20,B23,18,A22,17,D21,0\O,20,B24,18,A23,17,D22,0\H,21,B25,20,A24,18,D23,0\H,22,B26,21,A25,20,D24,0\H,23,B27,21,A26,20,D25,0\H,24,B28,20,A27,18,D26,0\H,21,B29,20,A28,18,D27,0\H,22,B30,21,A29,20,D28,0\H,23,B31,21,A30,20,D29,0\H,24,B32,20,A31,18,D30,0\B1=1.08558269\B2=2.49074872\B3=2.35455867\B4=1.36920803\B5=1.50918687\B6=1.51528916\B7=1.08959149\B8=1.09150522\B9=1.08829687\B10=1.08815096\B11=1.08229512\B12=1.08536892\B13=1.08677245\B14=1.08276266\B15=1.31319005\B16=2.52272104\B17=1.37280385\B18=2.03277742\B19=1.43085268\B20=2.36755405\B21=2.48742683\B22=1.51563793\B23=1.518588\B24=1.37917452\B25=1.08792891\B26=1.08791879\B27=1.08845532\B28=1.08824101\B29=1.08276288\B30=1.08586111\B31=1.08720092\B32=1.08425716\A1=145.54042378\A2=62.06665092\A3=33.14461498\A4=93.2553867\A5=35.08792603\A6=93.20337317\A7=108.20376787\A8=109.12191392\A9=107.0843763\A10=146.69330373\A11=109.09889229\A12=109.115964\A13=141.82162321\A14=93.16981694\A15=92.14710969\A16=108.9459844\A17=86.4911591\A18=109.34198261\A19=92.60278883\A20=62.26689634\A21=92.64883314\A22=111.55837656\A23=106.46543538\A24=94.56759008\A25=93.33542962\A26=109.07575222\A27=107.145684

25\A28=136.91277209\A29=145.77181992\A30=109.46573433\A31=109.72597725\D1=138.6610004\D2=-150.33563543\D3=-14.81454998\D4=-6.24402861\D5=-127.90314542\D6=-97.09911051\D7=120.77658774\D8=118.90183097\D9=3.81072115\D10=146.45100605\D11=-122.18191053\D12=-154.42208924\D13=90.19929584\D14=88.40079148\D15=135.83269349\D16=-121.66071794\D17=-100.96012\D18=171.98212427\D19=-95.91358971\D20=-114.34767255\D21=78.6706458\D22=-157.83001438\D23=-3.42480657\D24=93.70296958\D25=-91.33337466\D26=-171.27794695\D27=119.54533448\D28=-139.07556765\D29=151.40066977\D30=-55.09120416\\Version=EM64L-G03RevE.01\HF=-692.9966285\S2=0.764976\S2-1=0.\S2A=0.750095\RMSD=9.327e-09\RMSF=1.911e-05\Thermal=0.\Dipole=0.9460612,0.608951,-0.4356603\PG=C01 [X(C10H19O4)]\\@

BHandHLYP/cc-pVDZ

1\GINC-I7\FTS\UBHandHLYP\CC-pVDZ\C10H19O4(2)\SUZUKI\15-Jul-2011\1\#BHandHLYP/cc-pVDZ OPT=(TS,NoEigenTest,z-matrix,CalcHFFC,Maxcycle=100)NoSymm\\THP TS1 BHandHLYP/cc-pVDZ\\0,2\H\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\O,4,B4,3,A3,2,D2,0\C,4,B5,3,A4,2,D3,0\C,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,6,B8,4,A7,3,D6,0\H,7,B9,3,A8,2,D7,0\H,2,B10,1,A9,6,D8,0\H,3,B11,2,A10,1,D9,0\H,6,B12,4,A11,3,D10,0\H,7,B13,3,A12,2,D11,0\H,4,B14,3,A13,2,D12,0\H,4,B15,3,A14,2,D13,0\O,4,B16,3,A15,2,D14,0\O,17,B17,4,A16,3,D15,0\H,18,B18,17,A17,4,D16,0\C,18,B19,17,A18,4,D17,0\C,20,B20,18,A19,17,D18,0\C,21,B21,20,A20,18,D19,0\C,21,B22,20,A21,18,D20,0\C,20,B23,18,A22,17,D21,0\O,20,B24,18,A23,17,D22,0\H,21,B25,20,A24,18,D23,0\H,22,B26,21,A25,20,D24,0\H,23,B27,21,A26,20,D25,0\H,24,B28,20,A27,18,D26,0\H,21,B29,20,A28,18,D27,0\H,22,B30,21,A29,20,D28,0\H,23,B31,21,A30,20,D29,0\H,24,B32,20,A31,18,D30,0\\B1=1.09355848\B2=2.4912749\B3=2.35175461\B4=1.37113003\B5=1.50953131\B6=1.51555141\B7=1.09764793\B8=1.09946417\B9=1.09638765\B10=1.09634179\B11=1.09046046\B12=1.09313399\B13=1.09452349\B14=1.09096081\B15=1.32211631\B16=2.5271859\B17=1.37506308\B18=2.03973779\B19=1.43063572\B20=2.36551411\B21=2.48731476\B22=1.5159157\B23=1.51903602\B24=1.38137083\B25=1.09613674\B26=1.09615953\B27=1.09650453\B28=1.09598905\B29=1.09099202\B30=1.09374017\B31=1.09497652\B32=1.09191875\A1=145.62006662\A2=62.099922\A3=33.29889151\A4=93.27917672\A5=35.06098624\A6=93.1511956\A7=108.14284767\A8=109.09114916\A9=107.01108861\A10=146.68802604\A11=109.12842689\A12=109.12142948\A13=141.98262127\A14=92.64835232\A15=90.96483676\A16=109.18695166\A17=86.26063988\A18=109.08217411\A19=92.3995297\A20=62.28649902\A21=92.69099764\A22=111.65505476\A23=106.41308836\A24=94.52263804\A25=93.25943047\A26=109.05765394\A27=107.15856629\A28=137.13937623\A29=145.8923932\A30=109.52117811\A31=109.76439478\D1=138.74340684\D2=-150.23122993\D3=-14.84730029\D4=-6.20933973\D5=-127.9367921\D6=-96.99831253\D7=120.76012594\D8=118.8730033\D9=3.40814379\D10=146.70312314\D11=-122.33874363\D12=-155.06277482\D13=90.06358867\D14=88.00618125\D15=135.71308315\D16=-121.50135623\D17=-100.57954542\D18=171.66909002\D19=-95.92793893\D20=-114.31905636\D21=78.42181638\D22=-158.10380537\D23=-3.48441095\D24=93.51549582\D25=-91.33452942\D26=-171.57514587\D27=119.33966152\D28=-139.44676642\D29=151.50106544\D30=-55.41421692\\Version=EM64L-G03RevE.01\HF=-692.856735\S2=0.764828\S2-1=0.\S2A=0.75009\RMSD=8.800e-09\RMSF=1.019e-05\Thermal=0.\Dipole=0.8991645,0.6006694,-0.4272491\PG=C01 [X(C10H19O4)]\\@

BHandHLYP/aug-cc-pVDZ//BHandHLYP/cc-pVDZ

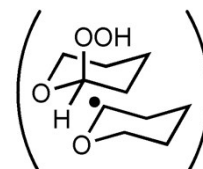
HF=-692.9040377

MPW1K/cc-pVDZ

1\GINC-I7\FTS\UmPW1PW91\CC-pVDZ\C10H19O4(2)\SUZUKI\21-Jul-2011\1\#mPW1PW91/cc-pVDZ IOp(3/76=0572004280) OPT=(TS,NoEigenTest,z-matrix,readFC,Maxcycle=100) Nosymm geom=check guess=read\\THP TS1 MPW1K/cc-pVDZ\\0,2\H\C,1,B1\C,2,B2,1,A1\C,3,B3,2,A2,1,D1,0\O,4,B4,3,A3,2,D2,0\C,4,B5,3,A4,2,D3,0\C,3,B6,2,A5,1,D4,0\H,3,B7,2,A6,1,D5,0\H,6,B8,4,A7,3,D6,0\H,7,B9,3,A8,2,D7,0\H,2,B10,1,A9,6,D8,0\H,3,B11,2,A10,1,D9,0\H,6,B12,4,A11,3,D10,0\H,7,B13,3,A12,2,D11,0\H,4,B14,3,A13,2,D12,0\H,4,B15,3,A14,2,D13,0\O,4,B16,3,A15,2,D14,0\O,17,B17,4,A16,3,D15,0\H,18,B18,17,A17,4,D16,0\C,18,B19,17,A18,4,D17,0\C,20,B20,18,A19,17,D18,0\C,21,B21,20,A20,18,D19,0\C,21,B22,20,A21,18,D20,0\C,20,B23,18,A22,17,D21,0\O,20,B24,18,A23,17,D22,0\H,21,B25,20,A24,18,D23,0\H,22,B26,21,A25,20,D24,0\H,23,B27,21,A26,20,D25,0\H,24,B28,20,A27,18,D26,0\H,21,B29,20,A28,18,D27,0\H,22,B30,21,A29,20,D28,0\H,23,B31,21,A30,20,D29,0\H,24,B32,20,A31,18,D30,0\\B1=1.09474809\B2=2.48196828\B3=2.34052833\B4=1.36757145\B5=1.50523204\B6=1.51129408\B7=1.09953796\B8=1.10086778\B9=1.09758319\B10=1.09764241\B11=1.09193824\B12=1.09427698\B13=1.09551529\B14=1.09257222\B15=1.32395291\B16=2.52472316\B17=1.36545885\B18=2.03779379\B19=1.42742599\B20=2.3538964\B21=2.47762139\B22=1.51173532\B23=1.51511069\B24=1.37782504\B25=1.09803845\B26=1.09747308\B27=1.09770901\B28=1.09710699\B29=1.09244957\B30=1.09493287\B31=1.09594177\B32=1.09371925\A1=145.79387712\A2=62.20015385\A3=33.44482695\A4=93.29286821\A5=35.11536453\A6=92.88097389\A7=108.13668968\A8=109.10592406\A9=106.9148871\A10=146.81603885\A11=109.10033936\A12=109.14090535\A13=14

2.07623168\A14=92.88840275\A15=91.39901869\A16=109.66761215\A17=86.05161919\A18=109.01245657\A19=92.41138267\A20=62.36124736\A21=92.73653644\A22=111.53718727\A23=106.47363552\A24=94.45849211\A25=92.99047437\A26=109.07861362\A27=107.21791788\A28=137.34947486\A29=146.13770945\A30=109.55409727\A31=109.60124749\D1=138.8374133\D2=-150.31698117\D3=-14.72763705\D4=-5.82566098\D5=-127.8222135\D6=-97.21954848\D7=120.80173665\D8=118.88480866\D9=2.83190702\D10=146.63169047\D11=-122.3777919\D12=-154.99193631\D13=90.04762781\D14=87.74109428\D15=135.63714928\D16=-121.21043224\D17=-100.26957633\D18=171.69930866\D19=-95.84763904\D20=-114.42284873\D21=78.41331016\D22=-157.89617517\D23=-3.62681318\D24=93.54703673\D25=-91.08062813\D26=-171.33884699\D27=118.99093507\D28=-139.79125889\D29=151.80231686\D30=-55.35551939\Version=EM64L-G03RevE.01\HF=-693.0790166\S2=0.762336\S2-1=0.\S2A=0.750067\RMSD=7.238e-09\RMSF=1.452e-05\Thermal=0.\Dipole=0.8987987,0.600858,-0.4061475\PG=C01 [X(C10H19O4)]\@

Complex of 2-hydroperoxytetrahydropyran and tetrahydropyran-2-yl radical (7b)



HF/6-311G**

1\1\GINC-I7FOptUHF\6-311G(d,p)\C10H19O4(2)\SUZUKI\07-Oct-2011\0\#HF/6-311G** OPT=(z-matrix,CalcFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THPooh-THPradical complex HF/6-311G**\0,2\O,0.1165519986,0.8518016076,-0.4698740112\C,-0.0305130228,1.1980269368,0.8925097218\C,2.414762982,0.0806552614,-0.1343885651\H,-1.0807652817,1.06585579,1.1166262041\H,2.2589420599,-0.9937725661,-0.2686062822\H,3.4072766893,0.3036809113,-0.5150018516\C,1.3912353903,0.8315029261,-0.9386904205\H,1.4134438705,0.7682631509,-2.0136705594\H,0.2177520632,2.2469852708,1.0250434625\C,0.8401089062,0.3334994481,1.7923649524\H,0.7237187575,0.6626641587,2.8212846399\H,0.499470091,-0.6989326878,1.7363657662\C,2.3024931078,0.4246416615,1.3538313901\H,2.6635171721,1.4354993867,1.5228639005\H,2.9233923956,-0.2435806235,1.9441069469\C,1.241386481,5.2553112806,2.6294799428\C,1.4177874061,5.3055154812,0.232661495\C,2.7066441879,7.0399324151,1.4815545268\C,1.8868950937,6.7508832284,0.2244646268\C,1.9157623099,6.6260461626,2.7272088479\O,0.6704470933,5.0181581641,1.3989895674\H,2.2592193941,4.6262956506,0.1553906673\H,3.6427255002,6.4962881863,1.4336630299\H,1.0180911267,7.4048646513,0.1876859005\H,1.1122576825,7.3424894448,2.8787562819\H,0.7452971674,5.1058955412,-0.5900882019\H,2.9495731577,8.0967201782,1.5451332985\H,2.4730233742,6.9375741447,-0.6711890316\H,2.5325934665,6.6519324478,3.6199164935\H,0.4282946206,5.1985949311,3.3393042682\O,2.0389120427,4.1851008785,3.067667652\O,3.2601145063,4.1624660779,2.4119063757\H,3.8752442145,4.1838905019,3.1259109609\Version=EM64L-G03RevE.01\HF=-689.2067914\S2=0.760265\S2-1=0.\S2A=0.750079\RMSD=4.998e-09\RMSF=1.845e-06\Thermal=0.\Dipole=1.0199922,1.0135516,0.7586934\PG=C01 [X(C10H19O4)]\@

BHandHLYP/6-311G**

1\1\GINC-I7FOptUBHandHLYP\6-311G(d,p)\C10H19O4(2)\SUZUKI\13-Oct-2011\0\#BHandHLYP/6-311G** OPT=(z-matrix,readFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THPooh-THPradical complex BHandHLYP/6-311G**\0,2\O,0.3249800639,1.424204777,-0.4303646572\C,0.0467514101,1.4321305948,0.9660408087\C,2.5387583623,0.4324394742,-0.0613936163\H,-1.0254746401,1.2999039137,1.0430720296\H,2.371173682,-0.5903494906,-0.4206579996\H,3.5708212676,0.6761417133,-0.2985479054\C,1.6323220039,1.3726419044,-0.7829546048\H,1.757863195,1.5386194715,-1.8402548516\H,0.3019885871,2.4091231417,1.3674035665\C,0.7969470438,0.3452592424,1.7089601259\H,0.5787646629,0.4323195105,2.7702709635\H,0.441945477,-0.6309361026,1.3813545581\C,2.2919346209,0.4700988354,1.4440622118\H,2.6502101068,1.4141852694,1.8471929501\H,2.8396417787,-0.3280561653,1.9377170459\C,1.2144805527,5.2403705322,2.7012311863\C,1.2002460774,5.0377320155,0.3093155829\C,2.715070252,6.7572386176,1.2729459785\C,1.7784299895,6.4236089631,0.1191374362\C,2.0005999583,6.5444955745,2.6053478136\O,0.5114751764,4.9359398905,1.5513728216\H,1.9763806366,4.2799271065,0.2556022728\H,3.5918743697,6.1216979702,1.2173301345\H,0.964190848,7.145123711,0.0779546699\H,1.2742562523,7.3426257126,2.7414823522\H,0.4555857193,4.8070830959,-0.4414371348\H,3.0551613562,7.787030494,1.2060485981\H,2.3028555127,6.4712291842,-0.8315686704\H,2.6888342447,6.6003436553,3.44340109\H,0.4660723809,5.3164193955,3.4827192795\O,1.9616453436,4.1450449577,3.1877117687\O,3.1459890473,3.9719300542,2.4269560367\H,3.8138806636,4.0291829774,3.1057301606\Version=EM64L-G03RevE.01\HF=-693.0112688\S2=0.755087\S2-1=0.\S2A=0.750019\RMSD=6.327e-09\RMSF=4.951e-06\Thermal=0.\Dipole=0.9273432,0.7786722,0.654633\PG=C01 [X(C10H19O4)]\@

BHandHLYP/cc-pVDZ

1\1\GINC-I7FOptUBHandHLYP\CC-pVDZ\C10H19O4(2)\SUZUKI\13-Oct-2011\0\#BHandHLYP/cc-pVDZ OPT=(z-matrix,readFC,Maxcycle=150) NoSymm freq=NoRaman geom=check guess=read\THPooh-THPradical complex BHandHLYP/cc-pVDZ\

0,2\O,0.3448336321,1.529139442,-0.3628662738\C,0.0839353077,1.4688062933,1.0355000873\C,2.5432822311,0.4678111176,-0.0672106426\H,-0.9976877951,1.3508108003,1.1198966249\H,2.3473022478,-0.5413010061,-0.4722345049\H,3.5848490223,0.6991880424,-0.3113969808\C,1.6485095791,1.4597957533,-0.7347428624\H,1.763169542,1.6653148428,-1.7953503105\H,0.3604914889,2.4261862226,1.4880257169\C,0.8213788611,0.3324253276,1.714892892\H,0.6108365219,0.3680915837,2.7886826726\H,0.4437774172,-0.6270333241,1.3395853891\C,2.3154162145,0.443855317,1.4410394767\H,2.6954264983,1.3719055197,1.8818234262\H,2.8599174652,-0.3883065864,1.8980502659\C,1.1771170406,5.2421892185,2.6770429982\C,1.1834495833,5.0286834155,0.2874020888\C,2.7231452013,6.7219942044,1.2577777881\C,1.7900996301,6.4026844436,0.0972746558\C,1.990342386,6.5298362774,2.582973325\O,0.4776410855,4.9446771906,1.5213894822\H,1.9514514347,4.2507779306,0.2432965456\H,3.5934535186,6.0627902111,1.2133748859\H,0.9847112299,7.1454530426,0.0474676145\H,1.2739082654,7.3490934042,2.7087231813\H,0.4386380617,4.8048649616,-0.4768084462\H,3.0900797315,7.750837261,1.1894451537\H,2.3252746026,6.4385360842,-0.8568146575\H,2.6737312354,6.5769361902,3.4355467848\H,0.4174541096,5.3373131482,3.4566807047\O,1.893980036,4.1334686043,3.1795811505\O,3.0794545891,3.9267178269,2.4232182108\H,3.7462860261,3.9812072381,3.1119155597\Version=EM64L-G03RevE.01\HF=-692.8701392\S2=0.755023\S2-1=0.\S2A=0.750018\RMSD=5.698e-09\RMSF=3.214e-06\Thermal=0.\Dipole=0.8925757,0.7123014,0.6302063\PG=C01 [X(C10H19O4)]\@

BHandHLYP/aug-cc-pVDZ//BHandHLYP/cc-pVDZ

HF=-692.9177599

MPW1K/cc-pVDZ

1\1\GINC-I7FOptUmPW1PW91\CC-pVDZ\C10H19O4(2)\SUZUKI\13-Oct-2011\0\#mPW1PW91/cc-pVDZ IOp(3/76=0572004280) OPT=(z-matrix,readFC,Maxcycle=100) Nosymm geom=check guess=read\THPooh-THPradical complex mPW1PW91/cc-pVDZ\0,2\O,0.3282186616,1.4660014357,-0.3986261721\C,0.072456533,1.4420714316,0.9963502953\C,2.530332411,0.434695351,-0.0704087762\H,-1.0103528631,1.3281678102,1.0885460166\H,2.3431608326,-0.5850734403,-0.4557258485\H,3.5716447878,0.6686486235,-0.3178861485\C,1.6324215,1.4027800606,-0.7586981901\H,1.7541622351,1.5961887132,-1.8222064505\H,0.3509798871,2.4124481188,1.4257101207\C,0.8092339475,0.3273185959,1.7027340085\H,0.5933288305,0.3852918741,2.7754534718\H,0.4363528987,-0.6426898948,1.3469082141\C,2.2990730178,0.4407650799,1.4328507837\H,2.6731375472,1.3811092473,1.8562847114\H,2.8486472773,-0.3778718131,1.9104011575\C,1.1993418854,5.2492376426,2.6880582162\C,1.2017376708,5.0357842547,0.3109731534\C,2.7171955821,6.7450916554,1.2678513435\C,1.7867264377,6.4139876994,0.1150034506\C,1.9927005912,6.5446167789,2.5908389751\O,0.4964774078,4.9465509997,1.5386709829\H,1.9832931925,4.2678906734,0.2694637887\H,3.5960447492,6.0948962542,1.2199734047\H,0.9694970953,7.1456272633,0.067094619\H,1.264139414,7.3545239596,2.7181337103\H,0.4625461013,4.797049478,-0.4564194547\H,3.0738557193,7.7787147887,1.1979187228\H,2.3166498366,6.4562967579,-0.8428324809\H,2.676257825,6.6039279755,3.444237327\H,0.4403354915,5.335240875,3.4722940169\O,1.929374833,4.1537634211,3.1858695435\O,3.1159232156,3.973080264,2.4390345417\H,3.7807614488,4.0786180638,3.1253309466\Version=EM64L-G03RevE.01\HF=-693.0881542\S2=0.754898\S2-1=0.\S2A=0.750018\RMSD=7.704e-09\RMSF=1.954e-05\Thermal=0.\Dipole=0.8858114,0.7445753,0.6280755\PG=C01 [X(C10H19O4)]\@