

A Novel Catalytic Pathway for Perfluoroacyl Peroxide Synthesis.

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Supplementary Materials

(Absolute energies and Cartesian coordinates of optimized structures)

<p># RB3LYP/6-31G* Opt Trifluoroperacetic acid.</p> <p>HF=-601.9033431 RMSD=3.587e-009 RMSF=5.203e-005 PG= C01 [X(C2H1F3O3)]</p> <p>0 1 C,-0.9750752201,0.1667034792,-0.0488680479 F,-1.492532078,-0.6640088519,0.8678695073 F,-1.4762433188,1.3870746826,0.1346524545 F,-1.3181934932,-0.2710564364,1.2690709034 C,0.5629048985,0.2172223997,0.085877257 O,1.2098589631,1.209357736,0.3206548691 O,1.0753318259,-1.0066076532,-0.0971108894 O,2.5122464687,-0.9945233416,0.0221533966 H,2.6762438792,-0.0374537525,0.2113062099</p>	<p># RB3LYP/6-31G* Opt Trifluoroacetic anhydride.</p> <p>HF=-977.1243902 RMSD=7.426e-009 RMSF=6.367e-005 PG=C01 [X(C4F6O3)]</p> <p>0 1 C,-2.0193878042,0.4699633757,-1.1418842737 F,-1.3344736679,0.9258605862,-2.2019812168 F,-3.1671032429,-0.0614887826,-1.5573356458 F,-2.2804359344,1.4999681567,-0.3223635921 C,-1.1886760695,-0.5993637438,-0.395442896 O,-1.5465643218,-1.7128987615,-0.1775296335 O,-0.0010118686,-0.0123841258,0.000214511 C,1.0765606478,-0.7704181141,0.4195699871 C,2.0721842888,0.1750950281,1.1305238913 F,3.1194267519,-0.5209962081,1.5675958448 F,1.473529089,0.7730673218,2.1720591458 F,2.4948485884,1.1196572049,0.2762239284 O,1.2480498611,-1.9342513358,0.2417668187</p>
<p># RB3LYP/6-31G* Opt <i>Bis</i>(trifluoroacetyl)peroxide</p> <p>HF=-1052.2596692 RMSD=3.215e-009 RMSF=7.219e-006 PG=C01 [X(C4F6O4)]</p> <p>0 1 C,2.9011878211,0.0742862956,0.0248666839</p>	<p># RB3LYP/6-31G* Opt Trifluoroacetic acid</p> <p>HF=-526.7823571 RMSD=3.709e-009 RMSF=3.709e-005 PG=C01 [X(C2H1F3O2)]</p> <p>0 1 C,0.3614247064,0.4031715104,-0.2608337171 F,-0.297071356,1.5748836831,0.2776499966</p>

F,3.4170572106,0.4970886022,1.124353848 F,2.9652183541,-1.4047728371,0.1581394257 F,3.613721361,0.2970551279,-1.0360889697 C,1.4352056604,0.4029985752,-0.1554823724 O,1.0672991661,1.224258435,-0.9359786702 O,0.6735022544,-0.2628748299,0.7701438951 O,-0.674380632,0.2502674476,0.7735713843 C,-1.4350332607,-0.4004234288,-0.1636436593 C,-2.901217653,0.0738924756,0.022804645 F,-3.6126423368,-0.2804160599,-1.0446980229 F,-2.9653988043,1.4020767342,0.177291855 F,-3.4182256632,-0.5150080142,1.1124660999 O,-1.066224101,-1.2088135445,-0.9570428477	F,1.4431314639,0.5349201859,0.5261443002 F,0.7618425064,0.1156146414,-1.4997824923 C,-0.5557846568,-0.7171941632,0.2753471279 O,-0.8528061883,-1.6991422497,-0.3518845984 O,-0.9564727024,-0.4243238811,1.5215687034 H,-1.5307327002,-1.1569016299,1.8170403934
# RB3LYP/6-31G* Opt Peracetic acid HF=-304.2076633 RMSD=8.262e-009 RMSF=1.280e-004 PG=C01 [X(C2H4O3)] 0 1 C,-1.7225029817,0.3653134087,0.5605356424 C,-0.3005653113,0.3296654728,0.0692149441 O,0.3849667839,1.2730941497,-0.2724893283 O,0.1666938348,-0.9425246941,0.0442199733 O,1.531365193,-0.9878851081,-0.4264373533 H,-1.7852238779,-0.054646451,1.5691903916 H,-2.0650891547,1.4005664007,0.5675210549 H,-2.3638498423,-0.2348930049,-0.0922424444 H,1.6883661391,-0.0223750143,-0.5853188541	# RB3LYP/6-31G* Opt Acetyltrifluoroacetyl anhydride HF=-679.4282532 RMSD=7.395e-009 RMSF=4.572e-00 PG=C01 [X(C4H3F3O3)] 0 1 C,1.5317598499,0.4174975803,0.1619224395 F,1.8042241754,0.3136466125,1.1504065265 F,2.5440323735,-0.1012985043,-0.8564027304 F,1.4160646569,1.7218742432,-0.4690928277 C,0.2178650958,-0.3272754594,-0.4945612053 O,0.1371530347,-1.2105181642,-1.2943230659 O,-0.789959147,0.2374958633,0.2317802433 C,-2.0057241867,-0.453064744,0.4728648177 C,-3.0652488315,0.5472891285,0.8373892017 O,-2.0963944998,-1.6416728643,0.4229611234 H,-3.9848597712,0.0210639986,1.0945379097 H,-3.2425695631,1.2232455791,-0.0060235609 H,-2.7297681854,1.1585715488,1.6813182805
# RB3LYP/6-31G* Opt Acetyltrifluoroacetyl peroxide. HF=-754.5656244 RMSD=7.630e-009 RMSF=1.775e-005 PG=C01 [X(C4H3F3O4)] 0 1 C,1.915508793,-0.0608532097,0.3653164434 F,2.6887875145,0.1155844805,0.7197040221 F,1.9051178256,-1.3633950527,0.6776074239 F,2.4325499479,0.6281679418,-1.38179233 C,0.4848567332,0.4601768176,-0.0676857209	

O,0.0313396404,1.4825168657,0.4855462008 O,-0.1090699198,-0.433162826,0.7714305456 O,1.3995312392,0.0507397832,1.1958977948 C,-2.3826835181,-0.2731820211,0.2601947168 C,-3.6915086586,0.2669390494,0.7798386061 O,-2.1678859508,-0.8512655775,-.7644753553 H,-4.5042202871,-0.2953037969,0.3171953399 H,-3.7767762572,1.3201701452,0.4907807579 H,-3.7529613887,0.2028075446,1.8686442629	
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