Supplementary Information (SI) for Inorganic Chemistry Frontiers.

Supporting Information

Experimental

Materials

Methane (99.99%) was obtained from Scientific Gases; ethane (99%) and propane (99%) were obtained from Aldrich. Trifluoroacetic anhydride (99%,) trifluoroacetic acid (99%), potassium permanganate and metal trifluoromethanesulfonates (min. 99%) were purchased from Sigma-Aldrich and used as received.

General procedure for the oxidation of CH_4

$KMnO_4$ (0.062 mmol) in a Teflon cup rested on a Teflon-coated magnetic bar was put into a 100 ml autoclave reactor (Parr) with a glass liner. A suspension of metal triflate (0.031 – 0.062 mmol) in 3.75 ml of a mixture of TFAA/TFA (4:1 by volume) was then charged into the autoclave reactor and the autoclave was closed and flushed 2 times with CH_4 (20 atm). The reactor was charged with CH_4 to the desired pressure (6-30 atm). The reactor was put into a water bath and set to the desired temperature (20-40 ^oC) for the reaction. After the mixture was stood for sufficient time to attain temperature equilibration, a strong magnet was used to attract the stir bar to topple the Teflon cup to introduce the $KMnO_4$ solids into the reaction mixture to start the reaction. The reaction mixture was then kept at the desired temperature for the appropriate time under vigorous stirring by a Teflon coated magnetic bar. At the end of the reaction, the reactor was immersed in an ice bath at 0-2 ^oC for 0.5 h. The excess CH_4 gas was released, and the resulting solution was taken out of the reactor. 1 µl of nitromethane was added to the resulting solution as an internal standard. The reaction products were identified by GC/MS (Aligent 5890) and quantified by GC (Aligent 5500) fitted with a HP5MS column and a FID detector. Temperature Program: Initial temperature: 30 ^oC, Initial Time: 6 minutes, Rate: 15 ^oC/min, Final temperature: 220 ^oC, Final time: 3 minutes.

Analysis of metal contents by ICP-AES was performed with a PerkinElmer Optima 6000 Spectrometer.

Table S1 Oxidation of methane by $KMnO_4$ in TFAA/TFA(4:1 by vol) in the presence of $Sc(OTf)_3$ under different pressure of CH_4.[a,b]

Pressure of CH_4 used	Percentage yield of methyl trifluoroacetate[c]
30 atm	18 %
20 atm	15 %
10 atm	13 %
6 atm	9 %
Blank (Air)	0 %

Conditions:
[a] $KMnO_4$ (0.062 mmol) and $Sc(OTf)_3$ (0.031 mmol) in mixture of 3 ml TFAA and 0.75 ml TFA (2.61M) stirred under different pressure of CH_4 at temperature 20-22 ^oC for 2.5 hour.
[b] Only methyl trifluoroacetate was found to be the product.
[c] % yield = 100 x (mol of CF_3COOCH^3/ mol of $KMnO_4$). Error ±2 %.

Investigation of the oxidation state of the manganese product after the oxidation

In a typical experiment, the resulting mixture after oxidation was added slowly to 10 ml of ice-cold water to convert TFAA to TFA (the reaction is vigorous). 10 ml of 2 M H_2SO_4 was added to the ice-cold solution, followed by the addition of 0.3 g of KI. The resulting brown solution was immediately titrated with standard sodium thiosulphate solution. A blank titration using the same amount of $KMnO_4$ (0.062 mmol) was also carried out.

Determination of carbon dioxide

The gas mixture after oxidation was flushed into a 125 ml sample flask until most of the gas inside the autoclave was released. 250 µL of the gas in the sample flask was injected into the GC fitted with a pack-column of RT-QPLOT and a thermal conductivity Detector (TCD) under a 30 ^oC isothermal condition. The retention time for CO_2 under this condition was 2.33-2.34 min. A calibration curve was obtained from flasks containing different known volumes of CO_2 (**Figure S1**).

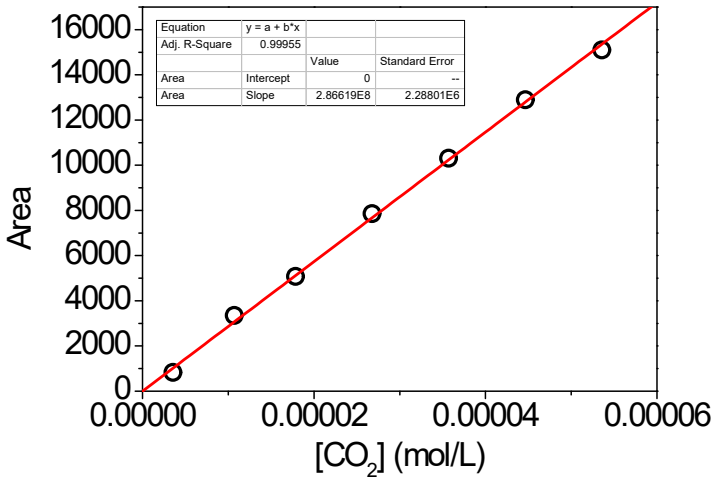


Figure S1 Calibration curve for CO_2. Area obtained from GC-TCD with 250 µL injection volume.

Experiment using Bromotrichloromethane ($BrCCl_3$) as a radical trap

The oxidation of CH_4 by $KMnO_4$ in TFA/TFAA with 0.5 equiv. $Sc(OTf)_3$ was carried out in the presence of 25 equiv. $BrCCl_3$. Bromomethane was detected by GC and identified by GCMS. The peaks for methyl trifluoroacetate and bromomethane in the GC were very close and could only be separated using GC (or GCMS) fitted with FFAP column. The program: Initial temperature: 30 °C, Initial Time: 6 minutes, Rate: 15 °C/min, Final temperature: 200 °C, Final time: 3 minutes.

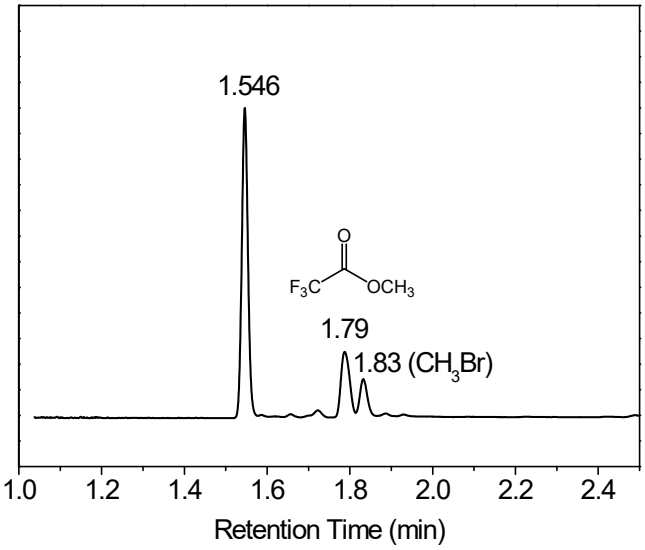


Figure S2 Gas chromatograph of methane oxidation with $KMnO_4$/TFAA-TFA/$Sc(OTf)_3$ in the presence of $BrCCl_3$ at room temperature using FFAP column.

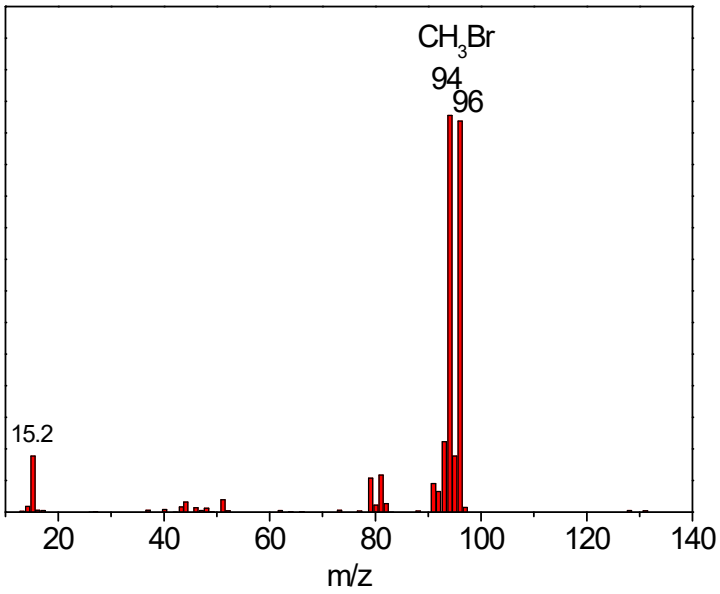


Figure S3 MS spectrum of species (CH_3Br) at GC retention time 1.83 min (FFAP Column).

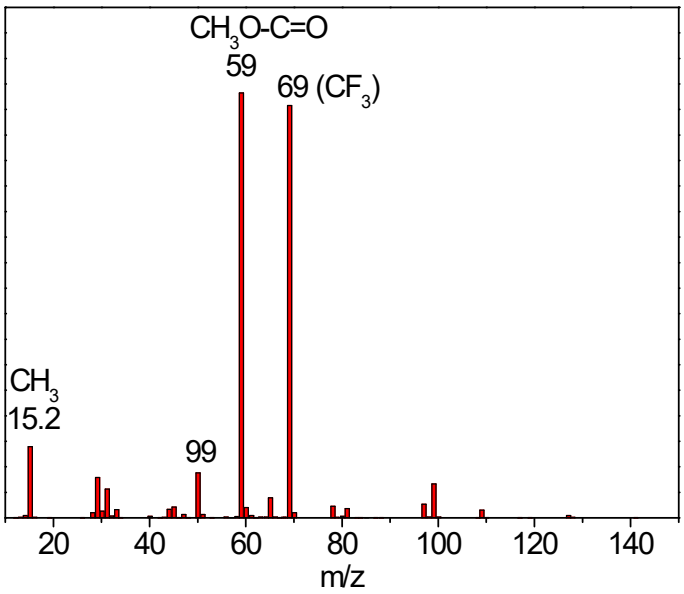


Figure S4 MS spectrum of species (methyl trifluoroacetate) at GC retention time at 1.79 min (FFAP Column).

Determination of kinetic isotope effects for CH_4 oxidation

The formation of CF_3COOCD_3 was confirmed by carrying out the oxidation using 30 atm of CD_4 to replace the CH_4 in the experiment (Figure S5, S6). Since CF_3COOCH_3 and CF_3COOCD_3 could not be separated using both HP5MS and FFAP columns, their relative amounts can only be found by using the integration results of the ions in GCMS from the reaction with a mixture of 15 atm CH_4/15 atm CD_4. The KIE was determined by ratio of the intensity of m/z 59(CH_3COO^+) and m/z 62 (CD_3COO^+) from GC-MS. The gas chromatographs and MS spectra of the product mixture are shown in Figure S7-S10.

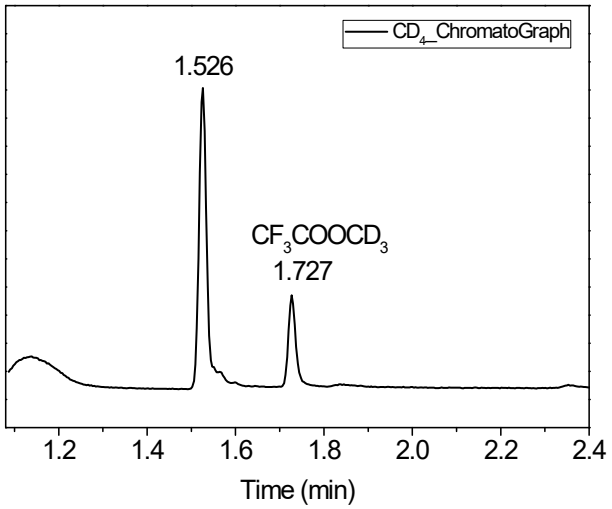


Figure S5 Gas chromatograph of resulting solution from methane oxidation with $KMnO_4$/TFAA-TFA/$Sc(OTf)_3$ under CD_4 (30 bar) atmosphere (FFAP polar column).

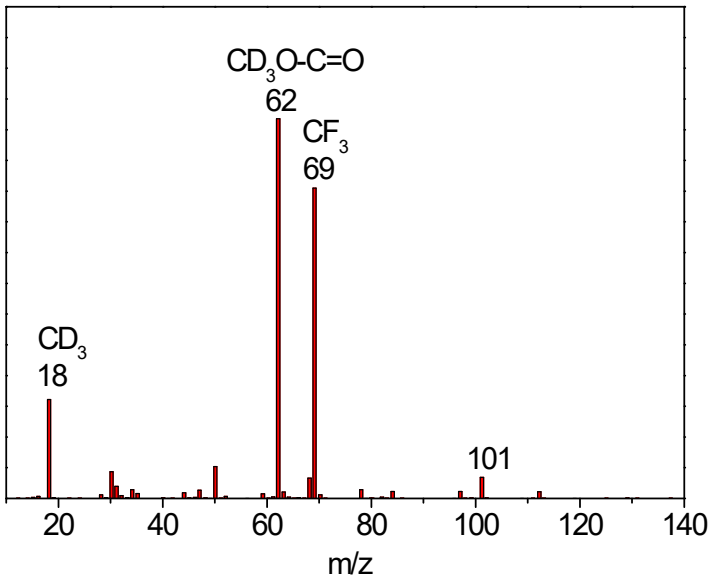


Figure S6 MS spectrum of product (CF_3COOCD_3) with GC retention time at 1.727 min of methane oxidation reaction with $KMnO_4$/TFAA-TFA/$Sc(OTf)_3$ under pure CD_4 (30 bar).

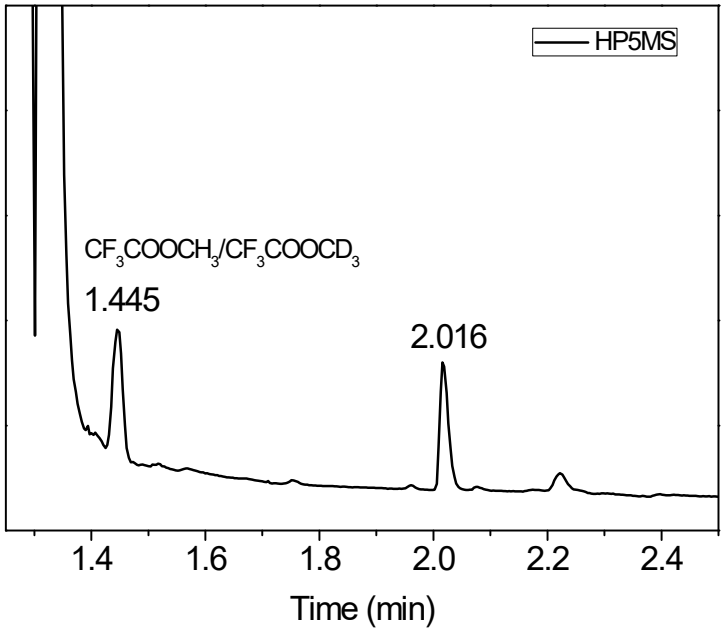


Figure S7 Gas chromatograph of resulting solution of methane oxidation with $KMnO_4$/TFAA-TFA/$Sc(OTf)_3$ under 15 atm of CH_4 and 15 atm of CD_4.

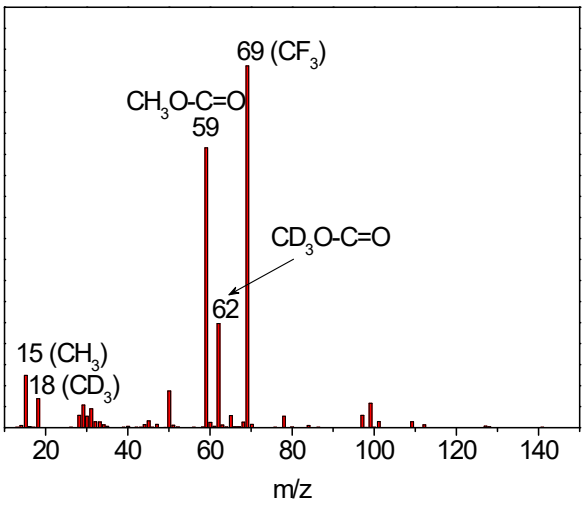


Figure S8 GC/MS of product (CF_3COOCH_3/ CF_3COOCD_3) with GC retention time at 1.65 min of methane oxidation with $KMnO_4$/TFAA-TFA/$Sc(OTf)_3$ under CH_4/CD_4 (FFAP polar column).

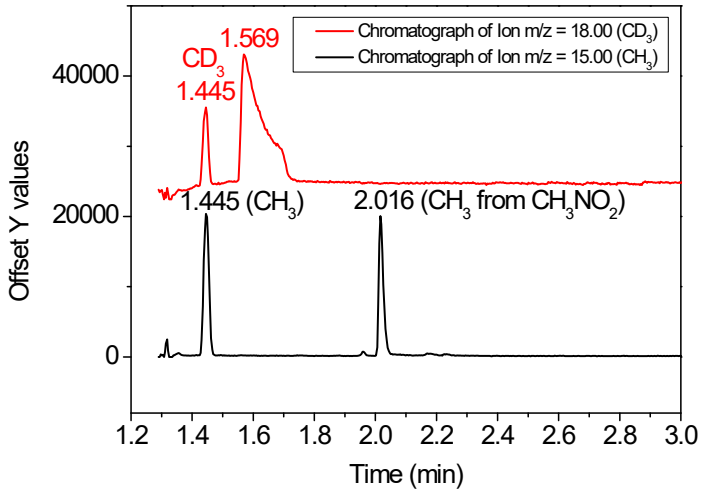


Figure S9 GC/MS of ion at m/z = 15 (CH_3) and 18 (CD_3) of product resulted from reaction of $KMnO_4$/TFAA-TFA/$Sc(OTf)_3$ with CH_4/CD_4. The m/z=18 at 1.569 is H_2O.

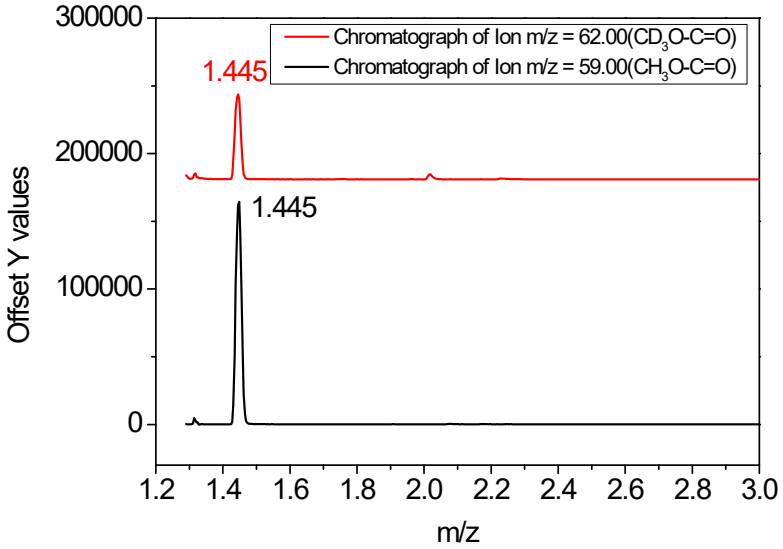


Figure S10 GC/MS of ion at m/z = 59 (CH_3O-C=O) and 62 (CD_3O-C=O) from reaction of $KMnO_4$/TFAA-TFA/$Sc(OTf)_3$ with CH_4/CD_4.

Computational details

The structures of all species were first optimized at the B3LYP-D3(BJ)/def2-SVPD level and vibrational frequencies calculations were subsequently performed to confirm the nature of stationary point.[1] All minimum structures do not have imaginary frequency while the transition state (TS) structures bear one imaginary frequency.[2] The solvent effect of methyl ethanoate ($CH_3CH_2COOCH_3$) was included by the polarizable continuum model (SCRF=PCM).[3] The actual solvent used in the experiment is trifluoroacetic anhydride (CF_3COOCF_3) but its dielectric constant (ε) is unavailable. We then used methylethanoate (ε = 6.8615) as the solvent in the calculations to mimic the solvent effect (see SI, Table S2) of CF_3COOCF_3. We have examined the effect of several selected solvents with different ε values to the barrier height ($\Delta G_{298}^{\ddagger}$) of **TS1($MnO_4^-$)** (for H-atom transfer) and **TS3(MnO_4^-)** (proton transfer) and found that no significant change in $\Delta G_{298}^{\ddagger}$ with the ε value. All the calculations were performed with Gaussian 16 package.[4]

The energy level of the highest occupied molecular orbitals (HOMO for the transition states, **TS1(MnO_4^-)**, **TS(4TFA)**, **TS1[$Sc(OTf)_2$]** and **TS1[$Sc(OTf)_2$/TFA]** in the HAT step were shown in Table S3. In each case, the HOMO is extensively delocalized on both the metal center and the methyl group, with the methyl group contributing significantly to each HOMO orbital. This suggests the cleavage of the H-CH_3 bond is a HAT, generating a radical $CH_3^\bullet$ and a formal Mn(VII) center *via* **TS1(MnO_4^-)**, **TS1(4TFA)** and **TS1[$Sc(OTf)_2$]** and **TS1[$Sc(OTf)_2$/TFA]**, respectively.

Table S2. The $\Delta G_{298}^{\ddagger}$ (in kcal/mol) for **TS1(MnO_4^-)** and **TS3(MnO_4^-)** at gas phase and in selected solvents (such as water, methanol, ethanol, quinoline, and chloroform).

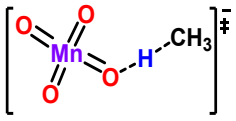
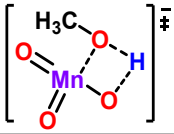
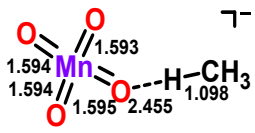
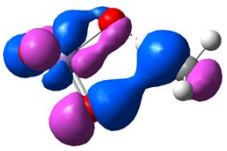
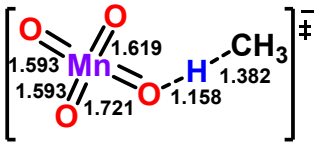
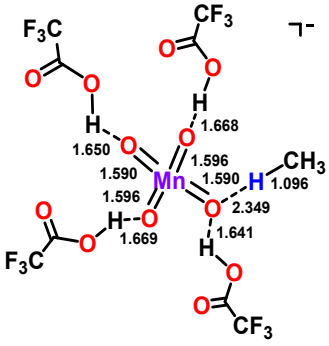
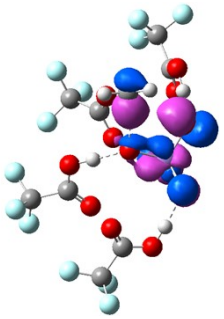
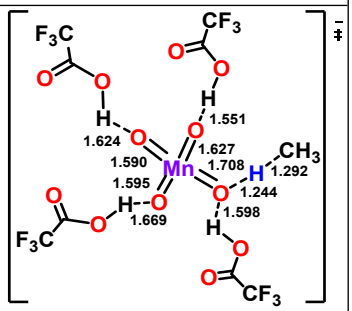
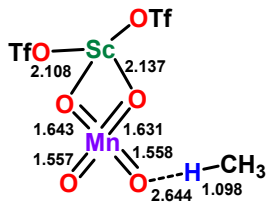
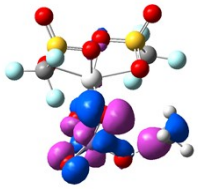
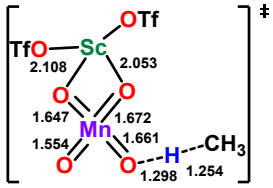
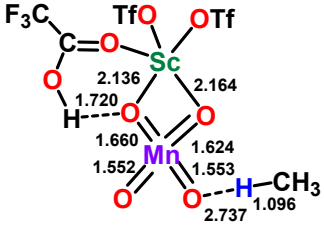
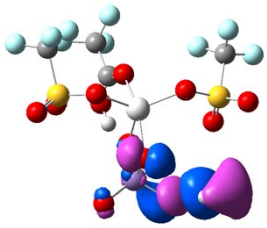
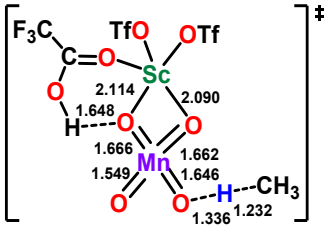
Solvent	TS1(MnO_4^-) (kal/mol) 	TS3(MnO_4^-) (kcal/mol) 
Methyl ethanoate(ε=6.8615)	**28.8**	**-1.1**
Gas phase	35.1	2.2
Water (ε=78.3553)	28.4	-2.9
Methanol (ε=32.613)	28.9	-0.3
Ethanol (ε=24.852)	28.4	-2.7
Quinoline (ε=9.16)	28.7	-1.6
Chloroform (ε=4.7113)	28.3	-3.2

Table S3. Spatial plots of the highest occupied molecular orbitals (HOMO), together with their orbital energies of the **TSs** in the HAT step, **TS1(MnO_4^-)**, **TS1(4TFA)**, **TS1[$Sc(OTf)_2$]** and **TS1[$Sc(OTf)_2$/TFA]**, and the corresponding structures of the **INT1** at B3LYP-D3(BJ)/def2-SVPD level.

	INT1	TS1 HOMO energy （a.u.）	TS1 $\Delta G_{298}^{\ddagger}$ (kcal/mol)
MnO_4^-		 -0.21385	 28.8
MnO_4/ 4TFA		 -0.26565	 20.4

$MnO_4/Sc(OTf)_2$		 -0.32246	 13.9
$MnO_4/Sc(OTf)_2$/ TFA		 -0.33734	 12.5

Reference:

[1] (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648−5652; b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785−789; c) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*,3297−3305; d) Schafer, A.; Horn, H.; Ahlrichs, R.; *J. Chem. Phys.* **1992**, *97*, 2571−2577; e) Schafer, A.; Huber, C.; Ahlrichs, R. *J. Chem. Phys.* **1994**, *100*, 5829−5835; f) Grimme, S.; Ehrlich S.; Goerigk, L. J. *Comput. Chem.* **2011**, *32*, 1456–1465; g) Goerigk, L.; Grimme, S. *Phys. Chem. Chem. Phys.* **2011**, *13*, 6670−6688.

[2] Gonzalez, C. and Gonzalez, H. B., *J. Phys. Chem.,***1990**, *94*, 5523-5527.

[3] (a) Miertuš, S.; Scrocco, E.; Tomasi, J. *Chem. Phys.* **1981**, *55*,117–129; b) Miertuš̃, S.; Tomasi, J. *Chem. Phys.* **1982**, *65*, 239−245.

[4] Gaussian 16, Revision A.03, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams-Young, D.; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa,

J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery, J. A. Jr., Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; and Fox, D. J. Gaussian, Inc., Wallingford CT, **2016**.

Path S1: $[MnO_4/TFA]^- + CH_4$

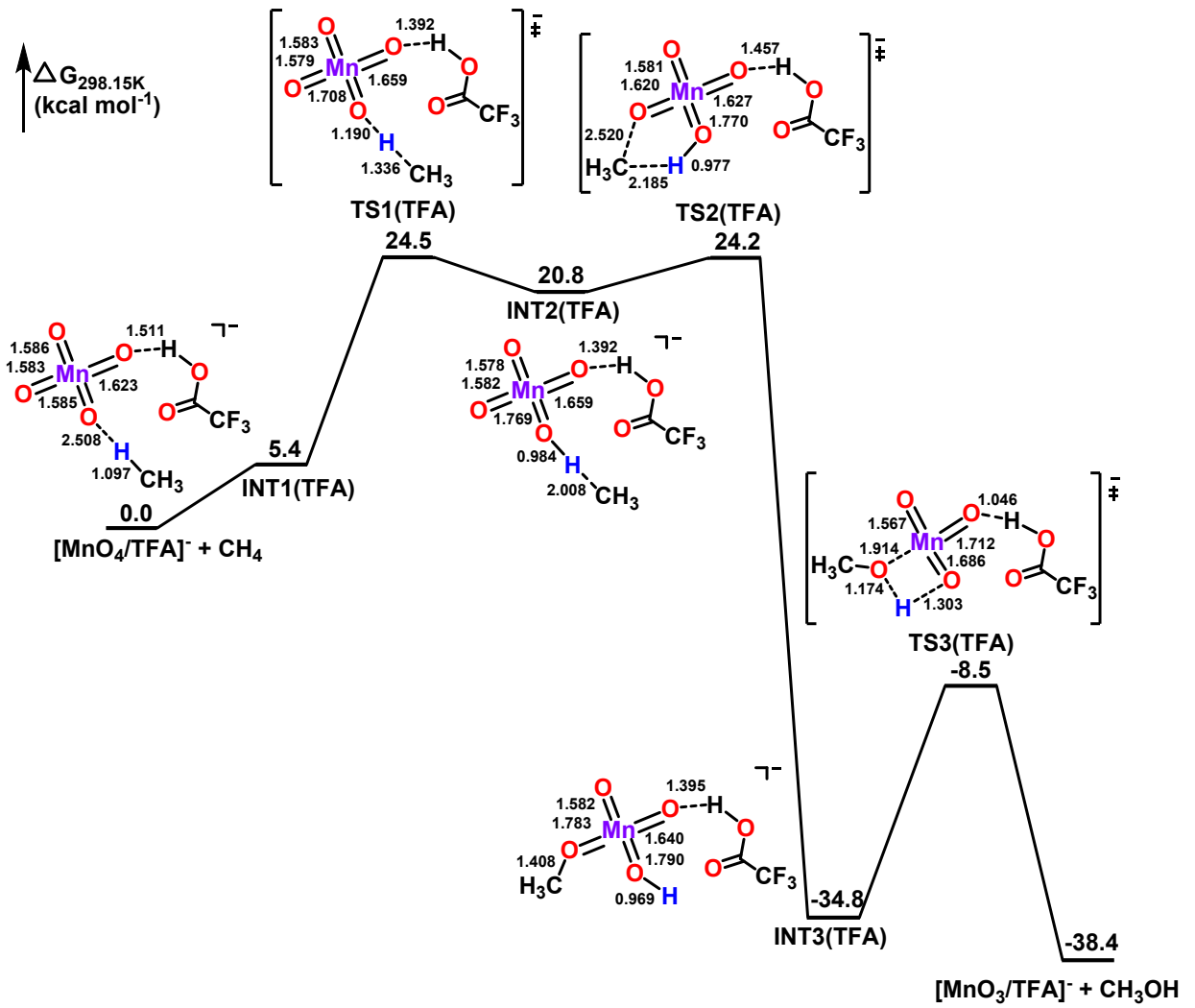


Figure S11. PES and structures for methane oxidation by $[MnO_4/TFA]^-$ at the B3LYP-D3(BJ)/def2-SVPD level. The relative 298.15 K Gibbs free energies in methylethanoate are given in kcal mol^{-1}.

Path S2: $[MnO_4/3TFA]^- + CH_4$

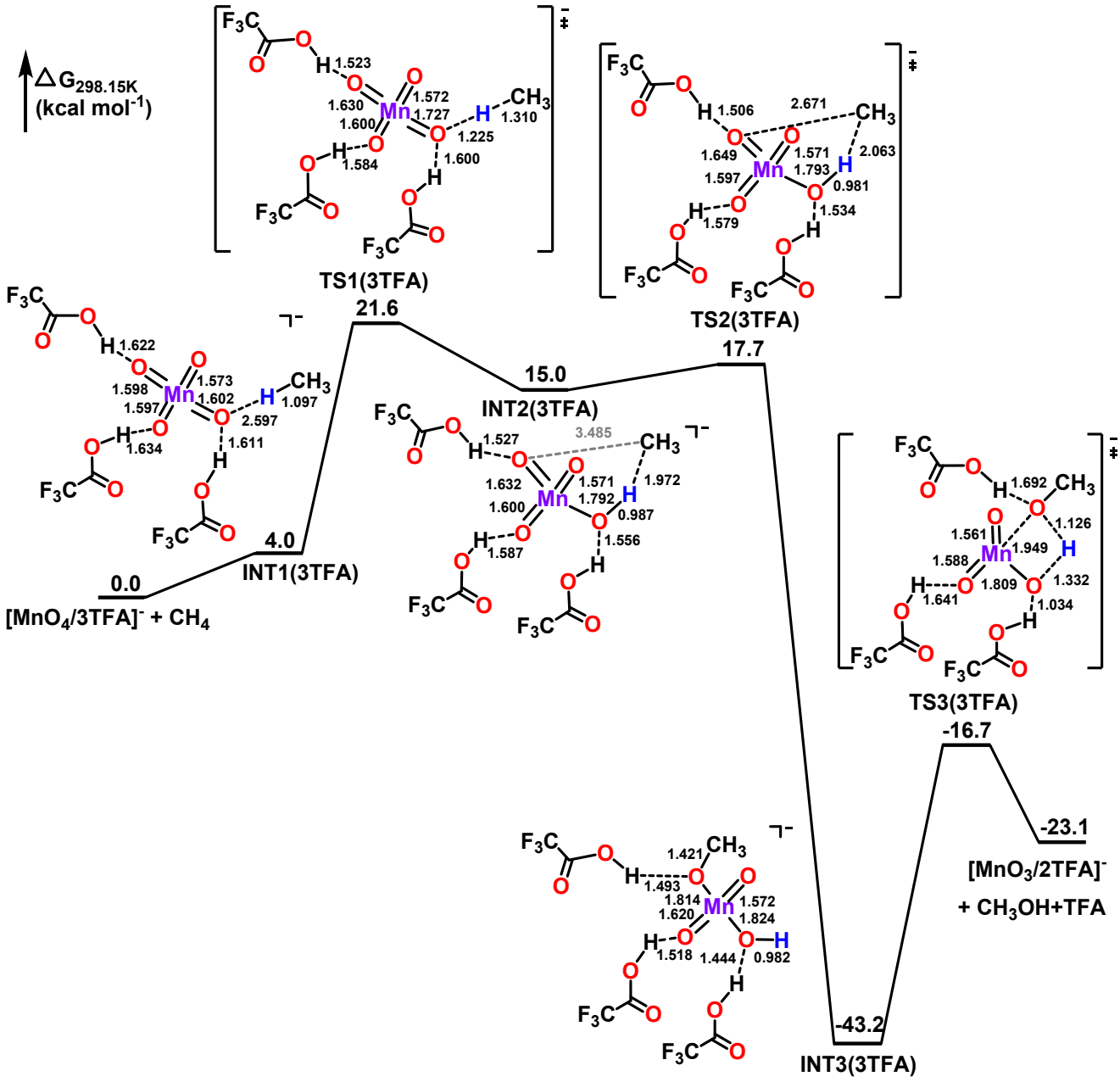


Figure S12. PES and structures for methane oxidation by $[MnO_4/3TFA]^-$ at the B3LYP-D3(BJ)/def2-SVPD level. The relative 298.15 K Gibbs free energies in methylethanoate are given in kcal mol^{-1}.

Path S3: $[MnO_4/3TFA]^- + CH_4$

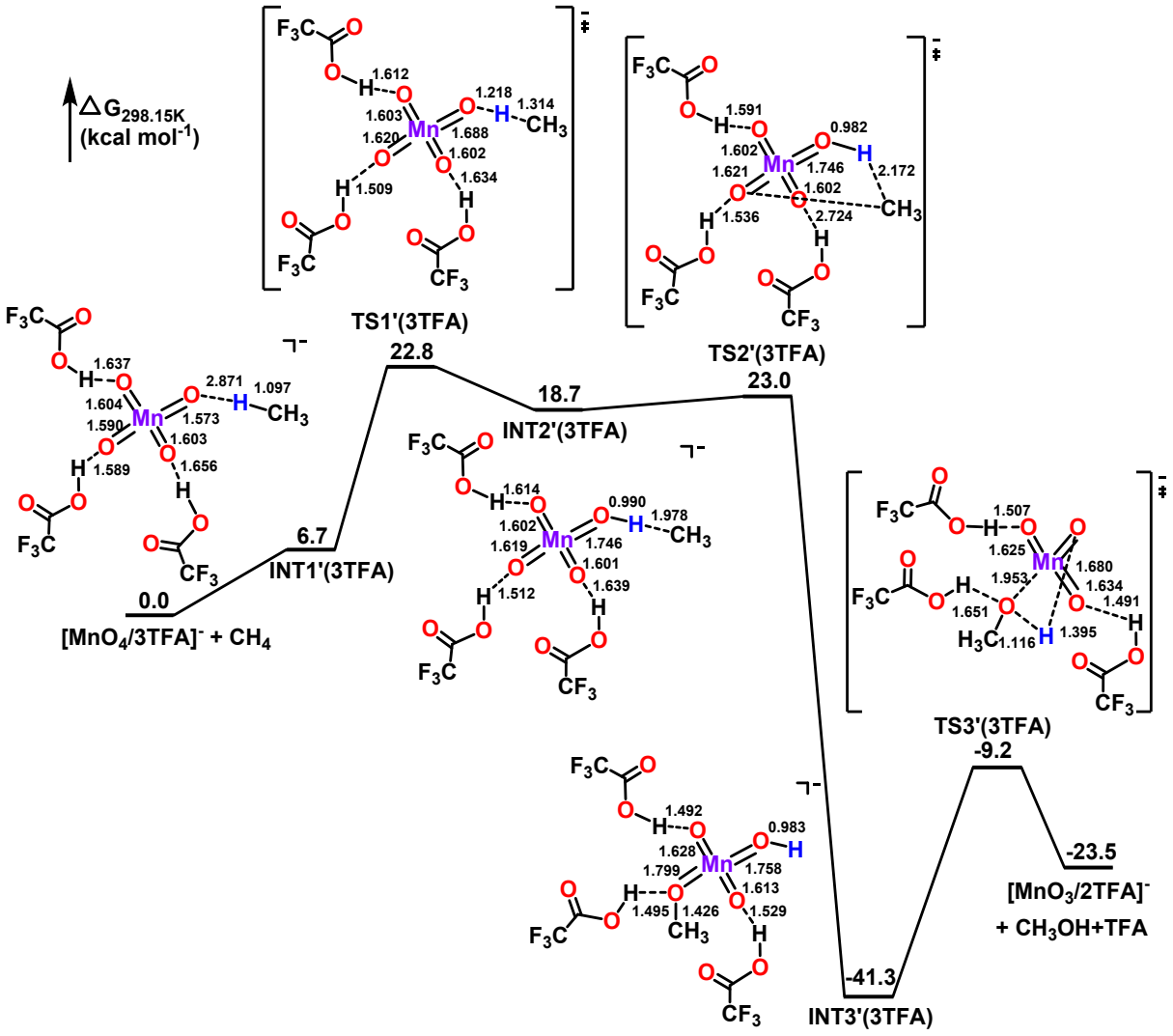


Figure S13. PES and structures for methane oxidation by $[MnO_4/3TFA]^-$ at the B3LYP-D3(BJ)/def2-SVPD level. The relative 298.15 K Gibbs free energies in methylethanoate are given in kcal mol^{-1}.

Path S4: $[MnO_4/Sc(OTf)_3]^-$ + CH_4

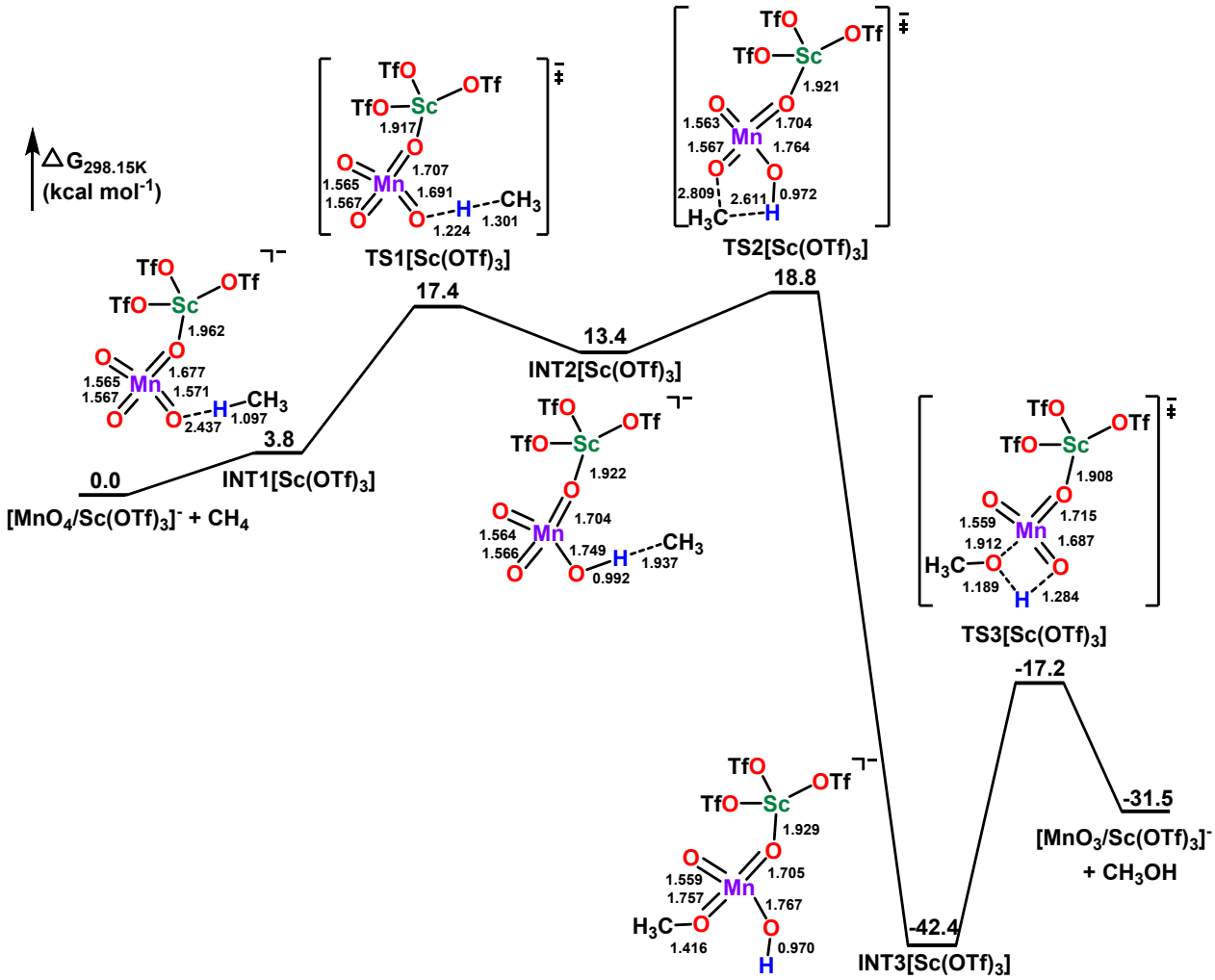


Figure S14. PES and structures for methane oxidation by $[MnO_4/Sc(OTf)_3]^-$ at the B3LYP-D3(BJ)/def2-SVPD level. The relative 298.15 K Gibbs free energies in methylethanoate are given in kcal mol^{-1}.

Path S5: $[MnO_4/Sc(OTf)_3]^-$ + CH_4

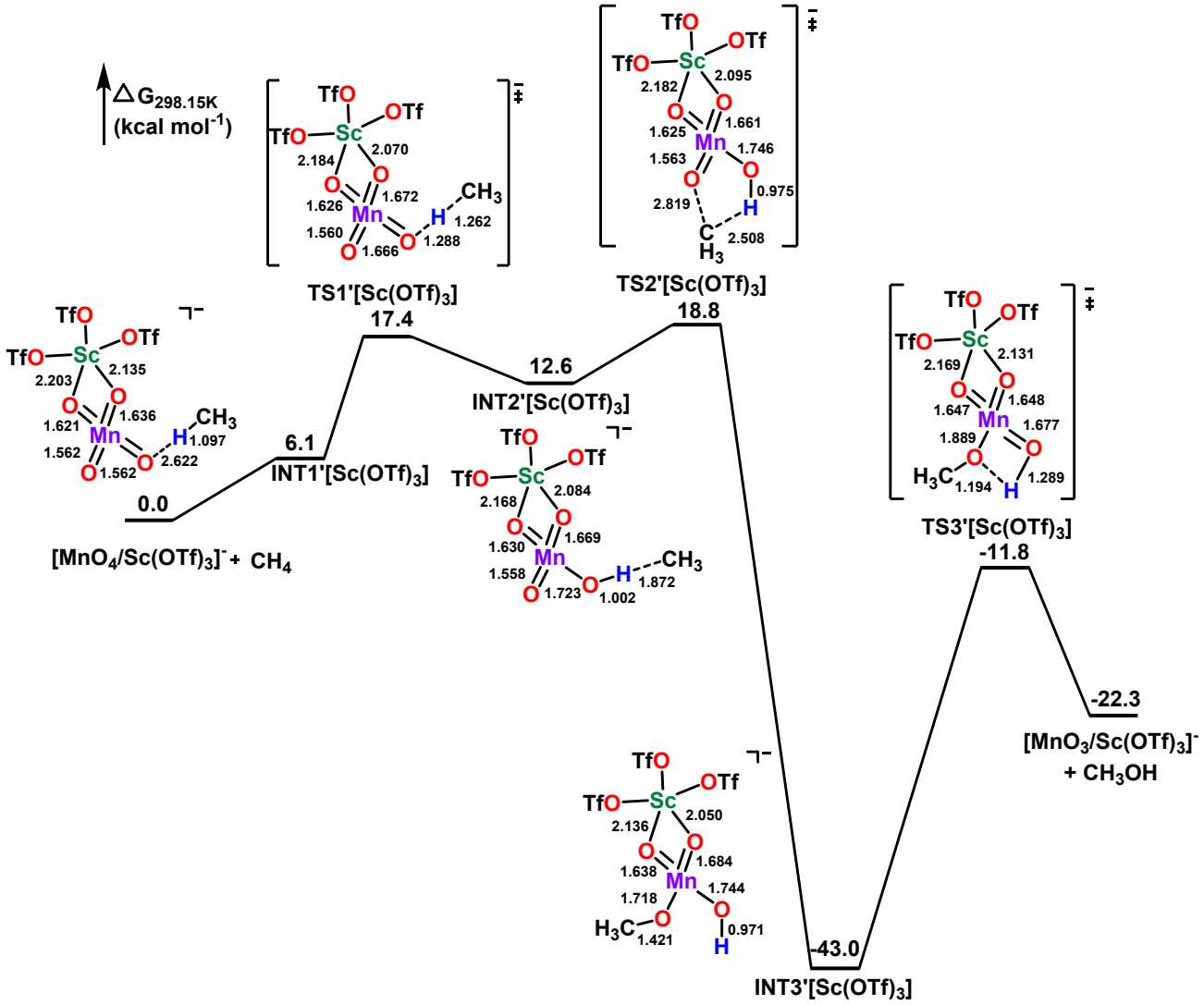


Figure S15. PES and structures for methane oxidation by $[MnO_4/Sc(OTf)_3]^-$ at the B3LYP-D3(BJ) /def2-SVPD level. The relative 298.15 K Gibbs free energies in methylethanoate are given in kcal mol^{-1}.

Path S6: $[MnO_4/Sc(OTf)_3/3TFA]^-$ + CH_4

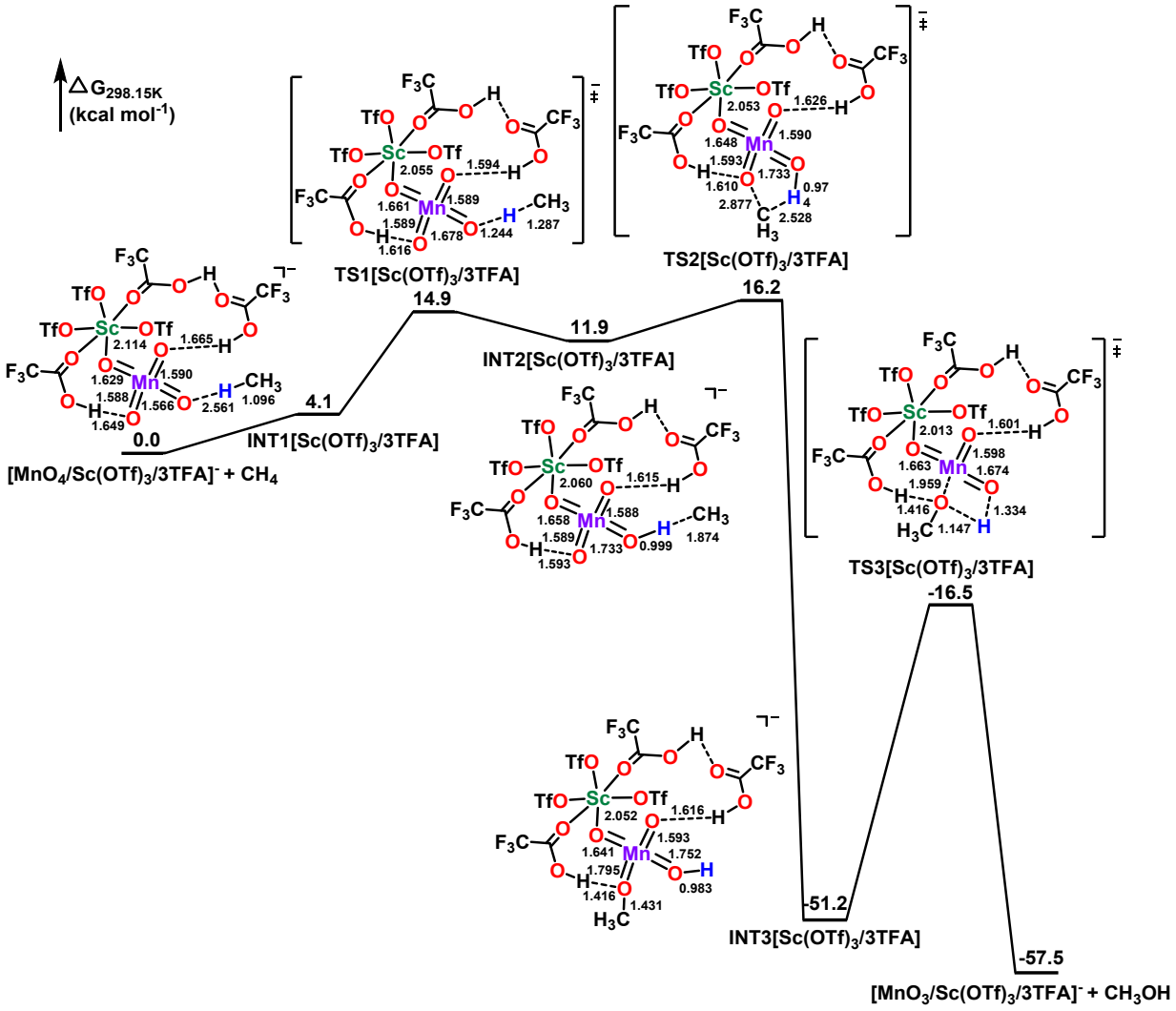


Figure S16. PES and structures for methane oxidation by $[MnO_4/Sc(OTf)_3/3TFA]^-$ at the B3LYP-D3(BJ)/def2-SVPD level. The relative 298.15 K Gibbs free energies in methylethanoate are given in kcal mol^{-1}.

Path S7: $[MnO_4/Sc(OTf)_2]$ + CH_4

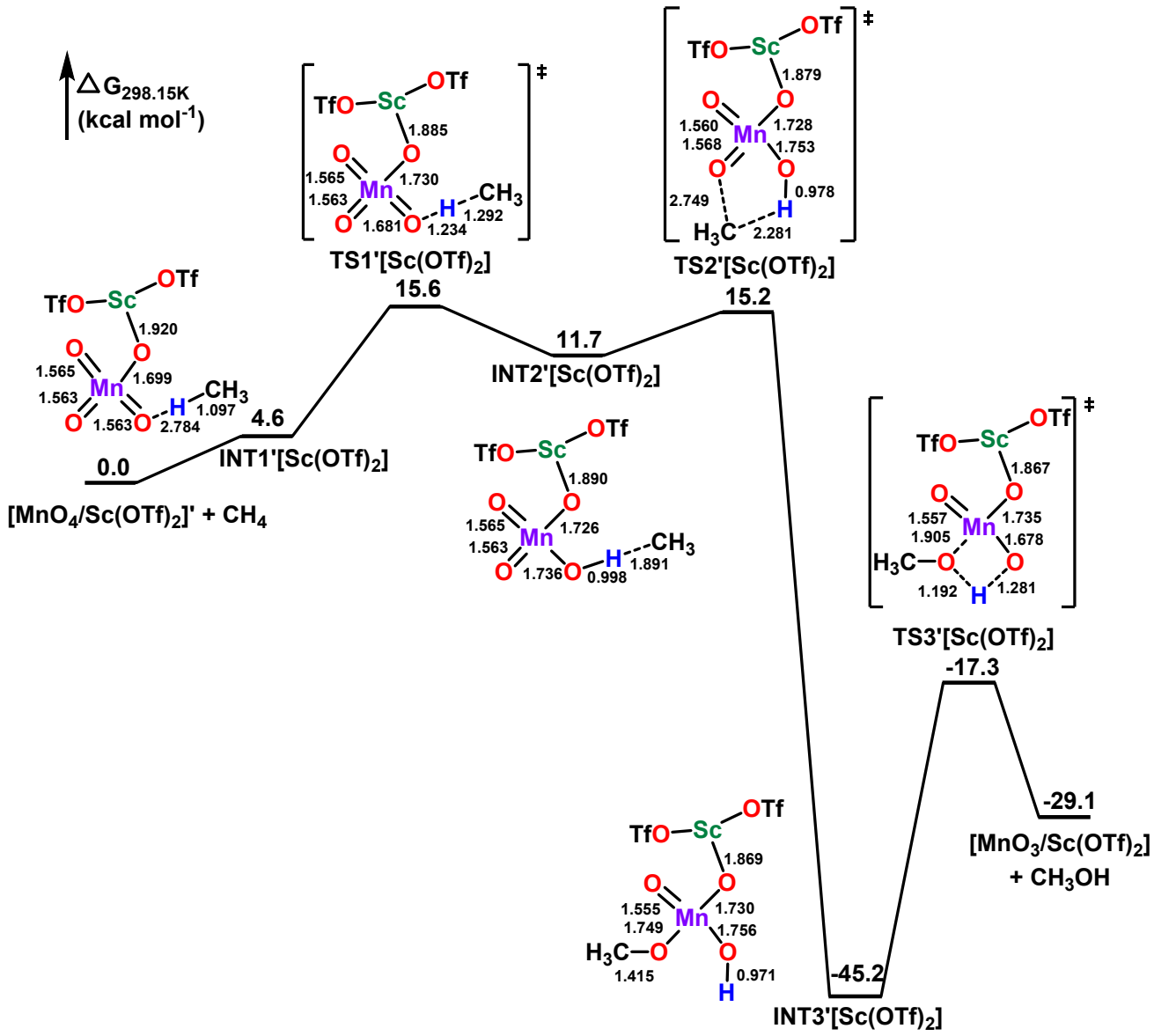


Figure S17. PES and structures for methane oxidation by $[MnO_4/Sc(OTf)_2]$ at the B3LYP-D3(BJ) /def2-SVPD level. The relative 298.15 K Gibbs free energies in methylethanoate are given in kcal mol^{-1}.

Path S8: $MnO_4/Sc(OTf)_2/3TFA] + CH_4$

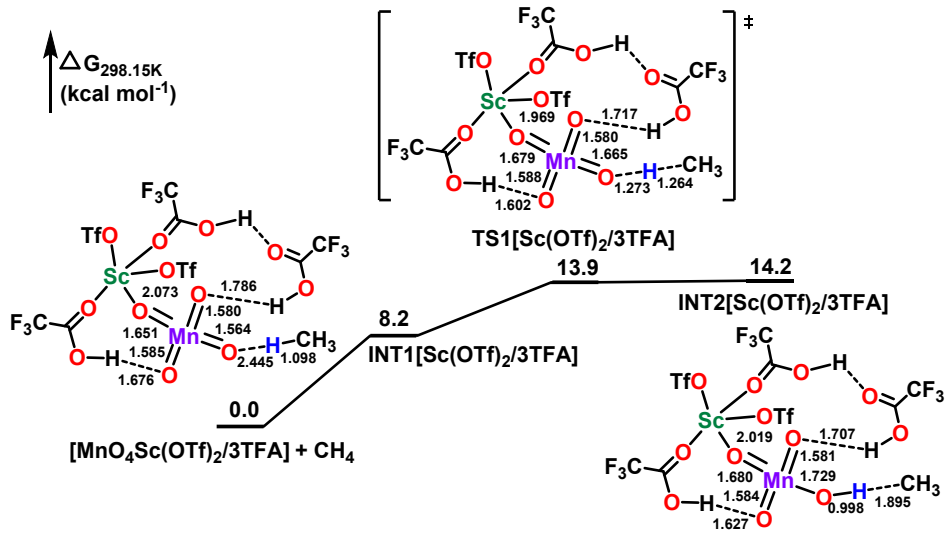


Figure S18. PES and structures for methane oxidation by $[MnO_4/Sc(OTf)_2/3TFA]$ at the B3LYP-D3(BJ) /def2-SVPD level. The relative 298.15 K Gibbs free energies in methylethanoate are given in kcal mol^{-1}.

Path S9: $[MnO_4/Sc(OTf)_2/3TFA] + CH_4$

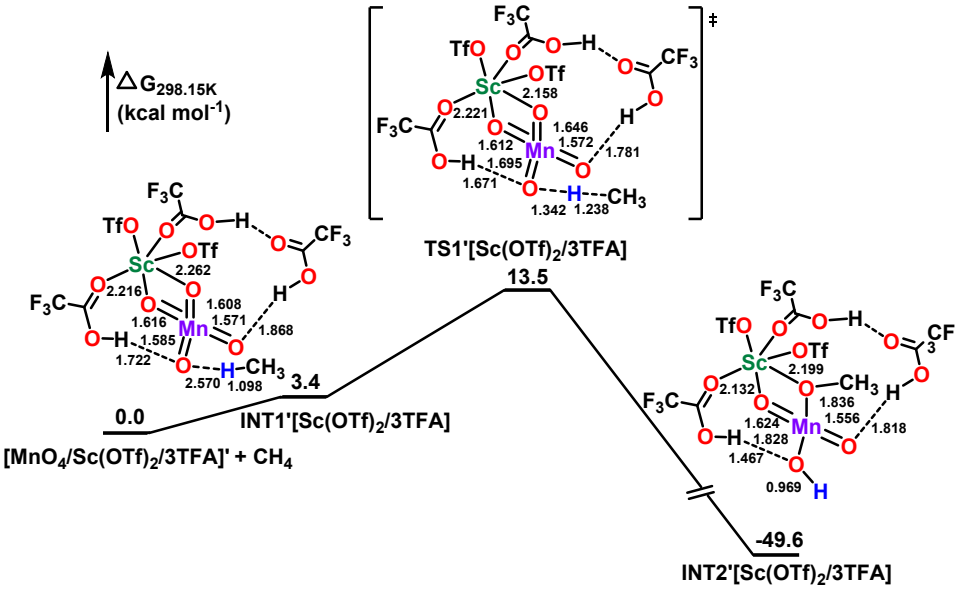
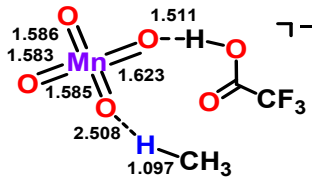
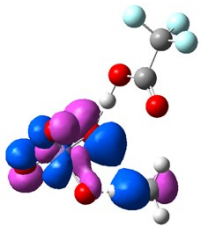
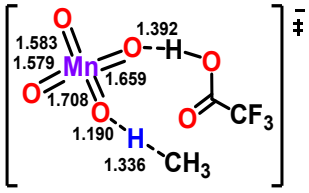
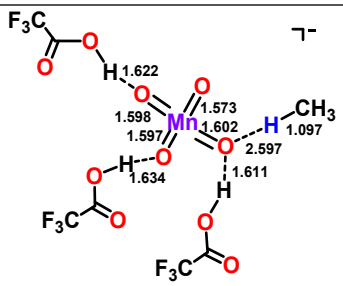
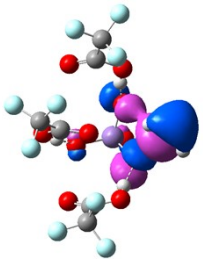
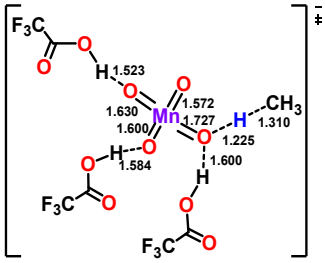
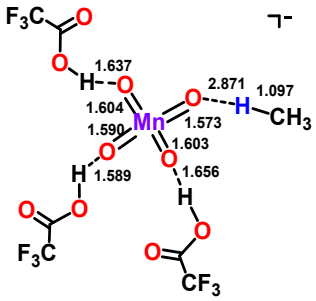
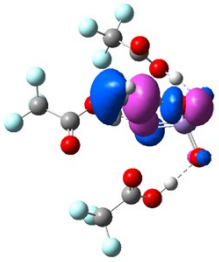
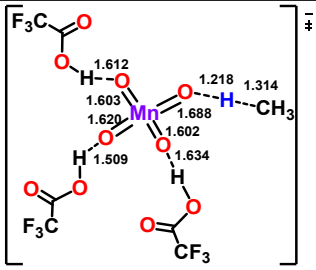
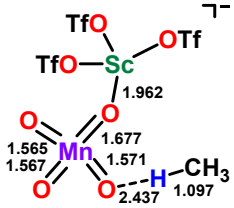
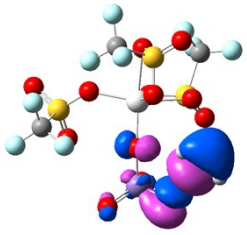
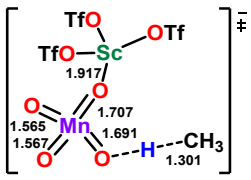


Figure S19. PES and structures for methane oxidation by $[MnO_4/Sc(OTf)_2/3TFA]$ at the B3LYP-D3(BJ) /def2-SVPD level. The relative 298.15 K Gibbs free energies in methylethanoate are given in kcal mol^{-1}.

Table S4. Spatial plots of the highest occupied molecular orbitals (HOMO), together with their orbital energies of the **TS1** in the HAT step, and the structures of the **INT1** at B3LYP-D3(BJ)/def2-SVPD level.

	INT1	TS1 HOMO energy （a.u.）	TS1 $\Delta G_{298}^{\ddagger}$ (kcal/mol)
MnO_4^-/ TFA		 -0.23858	 24.5
MnO_4^-/ 3TFA		 -0.27424	 21.6
MnO_4^-/ 3TFA		 -0.27139	 22.8
MnO_4^-/ $Sc(OTf)_3$		 -0.28304	 17.4

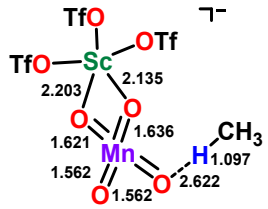
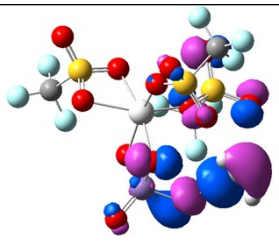
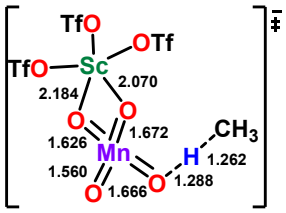
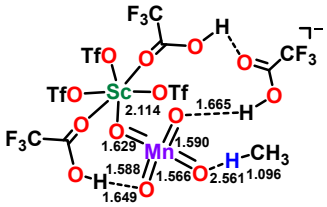
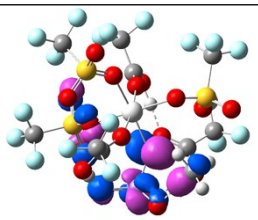
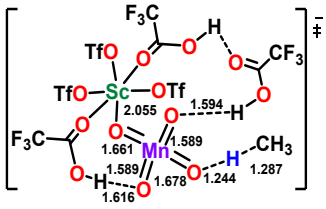
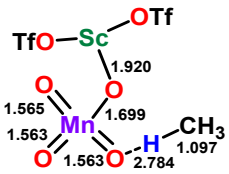
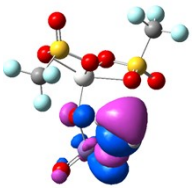
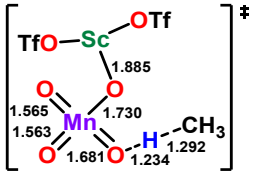
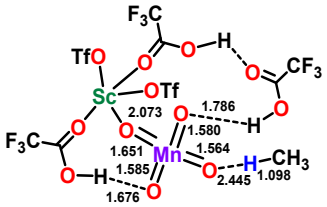
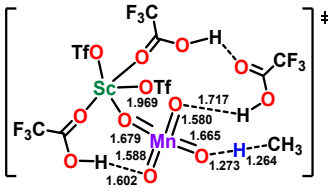
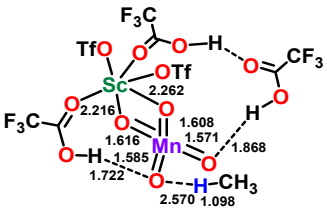
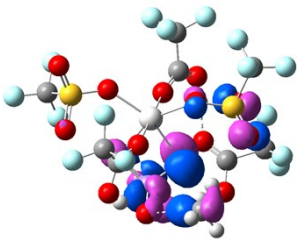
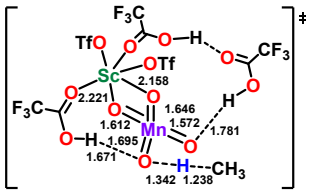
MnO_4^-/ $Sc(OTf)_3$		 -0.29748	 17.4
MnO_4^-/ $Sc(OTf)_3$/3TFA		 -0.29036	 14.9
MnO_4^-/ $Sc(OTf)_2^+$		 -0.30657	 15.6
MnO_4^-/ $Sc(OTf)_2^+$/3TFA		 -0.32256	 13.9
MnO_4^-/ $Sc(OTf)_2^+$/3TFA		 -0.33105	 13.5

Table S5. Cartesian coordinates of the optimized structures of all molecular species

CH_4

C	0.00000000	0.00000000	0.00000000
H	0.63388700	0.63388700	0.63388700
H	-0.63388700	-0.63388700	0.63388700
H	-0.63388700	0.63388700	-0.63388700
H	0.63388700	-0.63388700	-0.63388700

CH_3OH

O	-0.74833900	0.12336700	0.00000400
H	-1.15702300	-0.74989000	0.00001500
C	0.66698400	-0.02048100	0.00000200
H	1.09422800	0.99047000	-0.00119300
H	1.02389900	-0.55130000	0.89820100
H	1.02370100	-0.55332400	-0.89706700

(MnO_4^-)

O	1.41166300	-0.05953500	0.73911100
O	-1.16952600	-0.15114300	1.07311100
O	-0.09518700	-1.18722500	-1.05984700
O	-0.14717600	1.39785600	-0.75263800
Mn	0.00007200	0.00001500	0.00008400

(MnO_3^-)

Mn	0.00000000	0.00396700	0.00000000
O	1.58411400	0.20765300	0.00000000
O	-0.98434400	1.25953100	0.00000000
O	-0.59977000	-1.47958000	0.00000000

INT1(MnO_4^-)

O	-0.30178900	-0.32466600	-1.25237200
O	-0.28857300	0.24277900	1.28274400
H	-2.51209000	-0.02070200	0.27534600
O	1.48529400	1.31138000	-0.29689800
O	1.60937100	-1.22871800	0.26733500
Mn	0.62839000	-0.00009500	0.00005500
H	-4.19091700	0.05567800	0.90786500
H	-3.82430200	-0.91285400	-0.55704300
H	-3.76824000	0.87657500	-0.63308400
C	-3.57477100	-0.00042000	-0.00015500

INT2 (MnO_4^-)

O	-0.61013700	-0.08717200	-1.26474900
O	-0.31078300	0.04479800	1.34277700
H	-1.48745600	-0.07473600	-0.82940100
O	1.43056700	1.36984200	-0.14144700
O	1.48827700	-1.33803800	-0.01417500
Mn	0.62725900	0.00269200	0.01958300
H	-3.18149900	1.03077900	0.44085800
H	-3.15403300	-0.81715300	0.78394000
H	-3.80649900	-0.17604800	-0.86632300
C	-3.33923100	0.00907200	0.10035100

INT3(MnO_4^-)

H	-0.72438400	2.11764800	-0.00166300
Mn	-0.42103000	-0.15599300	0.00012600
O	-0.54156500	-0.95198500	1.37887200
O	1.12572500	0.77555000	-0.00204600
O	-1.36552400	1.39177900	0.00010800
O	-0.54496600	-0.95479300	-1.37675000
C	2.31593200	0.03216600	-0.00047300
H	3.17006600	0.73123200	-0.00468700
H	2.39866300	-0.60928700	0.89618700
H	2.39644900	-0.61716800	-0.89162900

TS1 (MnO_4^-)

O	-0.71211300	0.00126100	-1.14326100
O	-0.27748900	0.00013100	1.38165200
H	-1.72267600	0.00089700	-0.57707300
O	1.41512400	1.34514800	-0.13044600
O	1.41305800	-1.34640700	-0.13127200
Mn	0.57200300	-0.00004200	0.00301200
H	-2.97741300	0.91984200	0.63333000
H	-2.97605900	-0.92026000	0.63284000
H	-3.59303500	-0.00026500	-0.84596000
C	-2.95659000	-0.00003800	0.04469500

TS2 (MnO_4^-)

O	0.33959300	1.00920900	1.08283400
O	0.60060000	-0.73056700	-0.84619300
H	1.27862200	0.84767100	0.88514900
O	-1.46935600	0.90793000	-0.98599700
O	-1.40765600	-1.10300400	0.83070700
Mn	-0.60819300	-0.02575600	-0.02635700
H	3.13983700	-0.14407400	-1.17499700
H	3.16113700	-0.99988200	0.49894300
H	3.58332900	0.83421500	0.37429100
C	3.25607700	-0.09376200	-0.09587800

TS3 (MnO_4^-)

H	0.96286300	-1.18126500	-0.29920900
Mn	-0.57262800	0.05584700	-0.03062200
O	-0.41840700	1.51464000	-0.71461300
O	1.23224300	-0.53061400	0.49993700
O	-0.30067400	-1.27474400	-1.07323300
O	-1.62464500	-0.13968500	1.16942900
C	2.37463600	0.28898000	0.24249600
H	3.28093300	-0.29134800	0.46442500
H	2.38822300	0.62038200	-0.80514200
H	2.32773300	1.16539000	0.89835700

[MnO_4/TFA]$^-$

O	1.48920700	-0.28249600	-1.19417500
Mn	2.48758400	-0.02159200	0.06007300
O	3.23103600	1.36402000	-0.13391600
O	1.62795700	0.00910400	1.38914100
O	3.55521300	-1.19155500	0.13664600
H	0.02660300	-0.51303300	-0.85586400

O	-0.94320500	-0.73212900	-0.60865400
C	-1.63699300	0.32897400	-0.29906400
C	-3.08417400	-0.07786800	0.10433400
O	-1.28828000	1.48345100	-0.29669800
F	-3.68324600	-0.76849300	-0.88251000
F	-3.83086900	0.99659200	0.36861500
F	-3.07084300	-0.85665100	1.20096700

[MnO_3/ TFA]$^-$

Mn	1.87920400	-0.16320000	-0.00404300
O	1.92365700	1.62161800	0.08373700
O	2.39081100	-0.83310200	1.34020500
O	2.37669600	-0.70078700	-1.41142300
C	-2.34258500	-0.18491100	-0.00227100
C	-0.93369000	0.48559000	-0.01155500
O	-0.85274400	1.70320900	-0.01770600
H	1.01029900	1.96763200	0.06329400
O	-0.01038900	-0.40178200	-0.00002600
F	-2.46969200	-1.06307100	-1.01263000
F	-3.32235600	0.71795400	-0.11928000
F	-2.53650700	-0.85543200	1.14995900

INT1(TFA)

O	3.56863200	-1.28099600	-0.66894400
O	1.42092400	0.15956400	-1.08154900
O	1.57919600	-1.41264200	0.99241600
O	3.04598500	0.72318200	0.88782300
C	0.95635900	3.34985100	-0.21492300
H	0.09580300	2.91133600	0.30478000
H	1.82949600	2.70722300	-0.04656100
C	-3.19846000	-0.25435300	0.01916300
C	-1.69055800	0.12243100	0.09958600
O	-1.24658600	0.72423900	1.04536200
O	-1.06805000	-0.29893600	-0.96707000
H	-0.06614500	-0.07955900	-0.96502800
Mn	2.41369100	-0.46015600	0.04307200
F	-3.77765100	0.32767000	-1.04773400
F	-3.85388200	0.14304600	1.11193300
F	-3.35771700	-1.58393100	-0.10203500
H	1.15158900	4.35778900	0.17427600
H	0.74537900	3.40318100	-1.29099600

INT2(TFA)

O	-3.68432600	-1.12982300	0.63273600
O	-1.33415100	0.03327800	1.08883400
O	-1.63535300	-1.43445600	-1.09608200
O	-2.83429900	1.00241800	-0.84126800
C	-1.12716700	3.15703300	0.33888800
H	-0.27808400	2.63895600	-0.10474400
H	-2.28702300	1.71897500	-0.44661000
C	3.22029300	-0.20942600	-0.02645900
C	1.71495700	0.19119700	-0.03897900
O	1.30348700	1.00491700	-0.83585400

O	1.06929600	-0.44889200	0.88324300
H	0.02550300	-0.21954500	0.92889500
Mn	-2.39687900	-0.52178200	-0.05730600
F	3.78411400	0.09157400	1.15972000
F	3.90494300	0.43111500	-0.97864500
F	3.37202600	-1.53140600	-0.22627300
H	-1.65416600	3.92789000	-0.22278700
H	-1.35972600	3.00437000	1.39111300

INT3(TFA)

O	1.34397800	-0.49841500	1.40639200
O	2.39491500	-1.53758900	-1.05309200
O	3.77300300	0.42509000	0.44406700
H	1.90266000	-1.26353900	-1.84162400
C	-3.08956000	0.05462000	-0.03910000
C	-1.67429700	-0.56948800	0.14623100
O	-1.30473100	-1.47470500	-0.56710900
O	-1.04543100	0.02168600	1.11247300
H	-0.02131200	-0.27818000	1.22070800
Mn	2.35516600	-0.20992500	0.14768700
F	-3.80894200	-0.02640500	1.09629200
F	-3.77780100	-0.56308300	-1.00399100
F	-2.99545900	1.35749900	-0.36984600
O	1.46698900	0.86767900	-0.96080100
C	1.14605200	2.16313900	-0.51130900
H	0.53316800	2.65195100	-1.28550500
H	0.56764100	2.13976400	0.42724000
H	2.05555600	2.76643800	-0.34546200

TS1(TFA)

O	-3.61487700	-1.22666400	0.57647400
O	-1.31471400	-0.00209300	1.10321600
O	-1.56874200	-1.36142700	-1.15482700
O	-2.82023500	0.98482200	-0.74403300
C	-1.52059500	2.88392400	0.29512300
H	-0.48990500	2.62431600	0.04539500
H	-2.21135300	1.86398900	-0.22292500
C	3.23556600	-0.16451800	-0.03057900
C	1.73013100	0.23539600	-0.00432500
O	1.31643600	1.11232400	-0.72946100
O	1.08824700	-0.47548700	0.86763500
H	0.04499800	-0.24829100	0.93303600
Mn	-2.35891200	-0.51928500	-0.07774100
F	3.81592900	0.09712000	1.15767500
F	3.90493100	0.51113900	-0.96945200
F	3.38838500	-1.47778500	-0.27809400
H	-1.95568200	3.70869900	-0.27741800
H	-1.75798800	2.87853200	1.36092700

TS2(TFA)

O	3.83069500	-0.85715100	0.47758000
O	1.31267800	-1.58957100	-0.33002300
O	1.71514800	0.58303200	1.13219400
O	2.49249100	0.73211000	-1.30164400

C	1.05197500	2.90166800	0.40185300
H	0.96408700	2.93869600	1.48320900
H	2.11477200	1.56697200	-0.96303900
C	-3.16427100	-0.07204100	0.08845100
C	-1.68282800	-0.16339700	-0.38219500
O	-1.21446600	0.67836400	-1.11270100
O	-1.11869400	-1.22307600	0.11357100
H	-0.10673500	-1.32699900	-0.13478400
Mn	2.37621400	-0.41528900	0.04165600
F	-3.86954000	-1.13262900	-0.34924000
F	-3.75457000	1.03311700	-0.37522500
F	-3.24548800	-0.05297400	1.43107900
H	1.86154400	3.45355400	-0.07691200
H	0.21529000	2.53533500	-0.18987500

TS3(TFA)

O	-3.95306700	-0.66991100	-0.21205000
O	-1.35963200	-0.73408400	-1.28589900
O	-1.75941200	-0.51136000	1.53259200
H	-1.69692600	0.77833100	1.35598300
C	3.12836600	0.07296900	0.07467800
C	1.78758500	-0.68758000	-0.20332800
O	1.61699400	-1.76983900	0.35180200
O	1.03638800	-0.04483000	-0.99208800
H	-0.34587600	-0.50726900	-1.16059400
Mn	-2.43175000	-0.35469000	-0.00525500
F	3.82329300	0.27621800	-1.06773800
F	3.94131600	-0.58169900	0.91900000
F	2.89251800	1.29077700	0.61552300
O	-2.10923700	1.46373500	0.49720700
C	-1.22150200	2.31911400	-0.23123700
H	-1.63031300	2.48354600	-1.23544500
H	-1.16808700	3.27595100	0.30532000
H	-0.22215000	1.87233400	-0.30815000

[MnO_4/3TFA]$^-$

Mn	3.36892300	-0.00923400	0.50380000
O	2.15856600	-0.00378000	1.54171200
O	4.73897600	-0.01696800	1.27405100
C	-2.69573600	0.00650700	1.72706800
C	-1.23653400	0.00411200	1.19434300
O	-0.38745200	0.00148800	2.18487400
H	0.56009300	-0.00059800	1.86525800
O	-0.99927800	0.00473500	0.01139400
F	-2.92264800	1.09275100	2.48416600
F	-2.92726700	-1.08094300	2.48107700
F	-3.56805100	0.00978000	0.71957500
O	3.26580200	-1.31430500	-0.42095000
O	3.27916000	1.29837500	-0.41884900
O	1.00177100	-2.06465300	-1.50171100
H	1.88045800	-1.81474100	-1.08672600
C	0.16494200	-2.50889100	-0.59828300
O	0.36507500	-2.68290900	0.57721100
C	-1.19985200	-2.88525300	-1.24095800
F	-2.17152800	-2.88106300	-0.32375600

F	-1.11628500	-4.13394900	-1.74807700
F	-1.55153000	-2.06435200	-2.23452100
O	1.01822000	2.06240600	-1.49816100
H	1.89548600	1.80898200	-1.08240300
C	0.18162700	2.51023000	-0.59625000
O	0.38061900	2.68460000	0.57938200
C	-1.18082400	2.89078700	-1.24150300
F	-1.09154100	4.13832600	-1.75061300
F	-2.15387000	2.89207700	-0.32576600
F	-1.53422500	2.06963300	-2.23422400

[MnO_3/3TFA]$^-$

Mn	1.85307900	-1.27794200	1.83583400
O	1.12156100	-2.48100800	1.01723500
O	3.10166900	-1.57422300	2.74174700
C	-2.85679400	-1.64555100	-1.36545900
C	-1.38114300	-1.59988300	-0.87821300
O	-1.08705000	-2.57209400	-0.09311900
H	-0.11809500	-2.51940600	0.32422900
O	-0.65871800	-0.71651100	-1.31093500
F	-3.67591500	-2.22096500	-0.48240600
F	-2.91253100	-2.36139300	-2.50887400
F	-3.31138800	-0.41720700	-1.62850100
O	1.20835800	0.19687000	1.74620300
O	1.92463000	-0.32597400	-1.38515500
H	0.93123000	-0.45765800	-1.32237700
C	2.26926800	0.93394100	-1.29059300
O	1.55503200	1.90024700	-1.21668000
C	3.81869300	1.06075900	-1.28973000
F	4.19519500	2.33537600	-1.17698000
F	4.33494600	0.57194900	-2.43277000
F	4.35566700	0.37265700	-0.26866700
O	-0.73268500	1.73556700	1.17675400
H	0.02584300	1.08557500	1.39623400
C	-1.89633500	1.15652800	1.12135000
O	-2.17042600	-0.00273800	1.32533000
C	-2.99549000	2.18146500	0.72013500
F	-3.01646700	3.22298100	1.57113000
F	-4.20464700	1.61643500	0.72839700
F	-2.76642700	2.66187800	-0.51354400

INT1(3TFA)

Mn	1.12764900	2.98720900	-0.56261700
O	1.25459600	2.04045300	-1.84229900
O	1.43616400	4.47515500	-0.96967000
C	0.22743300	1.17030700	3.10327900
H	-0.69715600	1.39470000	3.64867800
H	1.03407500	0.94278900	3.81082900
H	0.06717000	0.31534600	2.43792700
H	0.51289100	2.03690600	2.49381000
C	-0.94573600	-2.24302400	-1.43409900
C	-0.21102700	-0.90620100	-1.14170700
O	0.17014200	-0.32022000	-2.24497200
H	0.64888100	0.53746600	-2.05092600
O	-0.01659700	-0.55173000	-0.00583900
F	-0.03549100	-3.23153200	-1.54530600

F	-1.65706500	-2.20923900	-2.56537400
F	-1.76953700	-2.55376600	-0.42817400
O	-0.35408500	2.88802300	0.02807400
O	2.17371900	2.51334800	0.55509500
O	-2.28127600	1.40477400	0.99701600
H	-1.53195000	1.91532500	0.57243900
C	-2.90327200	0.62879200	0.14961000
O	-2.71893400	0.51641700	-1.03664100
C	-3.98277200	-0.21001000	0.88998300
F	-4.64360800	-0.99477500	0.03847300
F	-4.87430900	0.59125300	1.50001900
F	-3.41691900	-0.98713100	1.82706800
O	2.78645600	0.08949100	1.31063700
H	2.58553500	1.01535800	0.97991400
C	2.92548100	-0.75987500	0.32616700
O	2.96050700	-0.53560800	-0.85707800
C	3.07228500	-2.20354700	0.88384400
F	4.22658800	-2.32439000	1.56801100
F	3.08254300	-3.09735200	-0.10654200
F	2.06662300	-2.51057800	1.71579100

INT2(3TFA)

Mn	0.38903500	3.10013900	-0.61316200
O	0.73296800	2.13511800	-1.84151200
O	0.69732100	4.62784500	-0.80857700
C	-0.41761600	1.40731900	2.96330400
H	-1.28096600	2.06571600	3.03763100
H	0.39699100	1.50827200	3.67868300
H	-0.45467200	0.54422200	2.30117900
H	0.61679400	2.28877500	1.53369200
C	-0.45235900	-2.45793600	-1.12789100
C	-0.06347700	-0.96570700	-0.94433900
O	0.19111300	-0.39030600	-2.08367900
H	0.44771500	0.57794400	-1.95316900
O	0.01304100	-0.49477200	0.16535100
F	0.66384000	-3.21398000	-1.06945000
F	-1.05374200	-2.70329600	-2.29607300
F	-1.26808900	-2.85481400	-0.14457400
O	-1.14772200	2.87789400	-0.11064500
O	1.27289000	2.52099100	0.83391300
O	-2.74964900	1.11296700	0.77012000
H	-2.09434800	1.76556000	0.33606100
C	-3.09043500	0.11980600	-0.00011800
O	-2.78795200	-0.07941900	-1.15169000
C	-3.99425400	-0.87732500	0.77964300
F	-4.36547200	-1.89738300	0.00476400
F	-5.10665400	-0.26564100	1.22605400
F	-3.34295400	-1.37454600	1.84484900
O	2.84879400	0.54533600	1.21556400
H	2.28196900	1.34097800	0.92848100
C	3.18292100	-0.23466600	0.22428300
O	3.01116700	-0.06516700	-0.95694000
C	3.86404000	-1.52504000	0.76181900
F	4.87419600	-1.23421700	1.59969200
F	4.35300600	-2.26235100	-0.23703100
F	2.97164100	-2.27349600	1.43521600

INT3(3TFA)

Mn	-0.12791100	-2.45114500	0.01986500
O	0.09530600	-1.36709300	-1.16341600
O	-0.54366800	-3.93050300	-0.31268300
C	1.20555300	-2.48631200	2.52885600
H	2.22206500	-2.60198500	2.93131300
H	0.61300600	-3.36989800	2.79988900
H	0.74543200	-1.59162500	2.97185700
H	-0.91504700	-0.88713000	1.51784700
C	0.40790800	2.93420300	0.86472900
C	0.19603300	1.41070900	0.64577400
O	0.27506500	1.11132700	-0.61108700
H	0.18725600	0.10485300	-0.80505900
O	0.01390000	0.67777300	1.59560900
F	-0.39633000	3.65809800	0.07266700
F	1.68019000	3.26773200	0.58105500
F	0.16294800	3.27584700	2.13178800
O	1.31453600	-2.36490400	1.11685700
O	-1.33205900	-1.70538300	1.17004200
O	2.85413100	-0.48131900	0.44871600
H	2.26081100	-1.29226300	0.68931000
C	3.58795900	-0.68646800	-0.60925500
O	3.68108700	-1.68831200	-1.27588400
C	4.39726900	0.59567100	-0.95838100
F	5.20396400	0.38918100	-2.00203900
F	5.15696400	0.98125200	0.08400600
F	3.57136100	1.61057800	-1.26244000
O	-3.52388300	-1.07888800	0.15133600
H	-2.60261400	-1.33731600	0.58962700
C	-3.60160400	0.19058100	-0.11567600
O	-2.78547500	1.05649300	0.10016200
C	-4.96395300	0.52722700	-0.78829500
F	-5.13550300	-0.18566000	-1.91557800
F	-5.04438000	1.82248100	-1.10211100
F	-5.98584300	0.23680000	0.03985900

TS1(3TFA)

Mn	0.55538600	3.07364800	-0.61757000
O	0.88626500	2.10635200	-1.84823100
O	0.78622000	4.60656900	-0.87789300
C	-0.01788000	1.82794900	2.67006400
H	-0.79692100	2.57759900	2.81769400
H	0.74845300	1.79196900	3.44904000
H	-0.36229500	0.85870100	2.30597500
H	0.69795800	2.27083900	1.66627900
C	-0.55724700	-2.41856800	-1.16977400
C	-0.08381000	-0.95285600	-0.97019400
O	0.18700800	-0.37568600	-2.10542600
H	0.50803600	0.57250100	-1.96671100
O	0.03874400	-0.50479000	0.14469800
F	0.51785500	-3.23412000	-1.13849300
F	-1.18669900	-2.61449200	-2.33246300
F	-1.37880000	-2.78729700	-0.18024200
O	-0.96023600	2.81665600	-0.07437400
O	1.46635100	2.58286000	0.76464700

O	-2.62795400	1.13770100	0.83940700
H	-1.94009000	1.75140300	0.39959800
C	-3.05572600	0.18846700	0.05714800
O	-2.78319100	-0.01259000	-1.10162300
C	-4.02708500	-0.74847500	0.83053300
F	-4.48702600	-1.72079800	0.04193200
F	-5.08217800	-0.05926700	1.30228400
F	-3.40557500	-1.31666500	1.87793100
O	2.84596900	0.43798500	1.22280200
H	2.37427700	1.27334600	0.90950400
C	3.12790500	-0.38093400	0.24349600
O	3.01512900	-0.19841300	-0.94179800
C	3.65655000	-1.72891800	0.80994800
F	4.71042200	-1.53360100	1.62216600
F	4.03632000	-2.54558900	-0.17397800
F	2.69737800	-2.34713600	1.52007100

TS2(3TFA)

Mn	-0.29083100	2.92627600	-0.44654200
O	-0.33720900	1.74463600	-1.51965400
O	-0.21337300	4.40454300	-0.96517400
C	-0.70348200	1.88850300	3.05742900
H	-1.75517100	2.13870200	3.16044000
H	0.03378600	2.52617100	3.54498400
H	-0.41774500	0.90373700	2.69144800
H	0.61094000	2.42969500	1.56262600
C	0.19387900	-2.78473200	0.01501600
C	0.06165400	-1.23693100	-0.02785300
O	-0.40982700	-0.81983200	-1.17066300
H	-0.36916900	0.18802300	-1.25372600
O	0.41815300	-0.58091100	0.91984200
F	1.47437500	-3.11714000	-0.24528900
F	-0.58242700	-3.40828000	-0.87657700
F	-0.11088400	-3.24816400	1.23313000
O	-1.50396200	2.73665800	0.65465300
O	1.04851200	2.63352100	0.70864500
O	-2.66098300	0.48997200	0.80195300
H	-2.23043500	1.41773500	0.69621900
C	-3.36376900	0.12243500	-0.23332500
O	-3.58644000	0.73272600	-1.24936300
C	-3.95368000	-1.29784300	0.00135500
F	-4.49980700	-1.78504300	-1.11339000
F	-4.90935600	-1.25202400	0.94942100
F	-3.00808600	-2.15936700	0.41514900
O	3.09681600	1.12245400	0.64657100
H	2.27237800	1.72097000	0.55933800
C	3.20509800	0.25002800	-0.31620100
O	2.53346500	0.14046000	-1.31222200
C	4.37666500	-0.73039000	-0.02388500
F	5.52880300	-0.06498200	0.17383600
F	4.55760700	-1.57996000	-1.03663000
F	4.12163900	-1.44972400	1.08371600

TS3(3TFA)

Mn	-0.63363700	2.61167600	-0.52512300
O	-0.72838000	1.34392700	-1.47695800

O	-1.00354300	4.04797600	-1.01109600
C	-2.32566700	2.94284700	1.89210700
H	-3.24981900	2.96461100	1.30721900
H	-1.91372400	3.95257100	2.00068600
H	-2.51159200	2.49987000	2.87773900
H	-0.28642900	2.21457600	1.43322800
C	0.98938200	-2.82269000	0.22997100
C	0.50192200	-1.35617300	0.07399700
O	0.02481900	-1.16252400	-1.12825100
H	-0.23468600	-0.20558600	-1.25837600
O	0.55228600	-0.57660800	0.99138200
F	1.82538800	-3.17754900	-0.75506300
F	-0.06677900	-3.66144300	0.19693600
F	1.61598600	-2.99671600	1.39494700
O	-1.38167400	2.09935700	1.19980200
O	0.72929400	2.60611900	0.66502100
O	-2.41193800	-0.35428000	0.85673900
H	-1.97544200	0.52261000	1.04172100
C	-3.50335000	-0.19468500	0.14563200
O	-4.00634700	0.83958100	-0.21153600
C	-4.11726400	-1.57833900	-0.20537900
F	-5.22501400	-1.43626800	-0.93328200
F	-4.43338900	-2.25074800	0.91539900
F	-3.24398600	-2.32072700	-0.90248900
O	3.07727600	1.72940300	0.44970500
H	1.68654500	2.26103900	0.47913600
C	3.28729800	0.76055200	-0.32703500
O	2.63655500	0.36019300	-1.29385000
C	4.55852700	-0.09128100	0.00603300
F	5.32272500	0.42352900	0.98495200
F	5.35230100	-0.23796200	-1.07702200
F	4.19434600	-1.33413000	0.40085600

INT1′(3TFA)

O	-1.60553100	-3.16442000	-0.82058500
O	1.01215700	-3.41571600	-0.81178900
O	-0.12596900	-1.38959300	0.34276700
O	-0.34811600	-3.75692400	1.37708500
C	4.04138200	0.33832600	-0.54325800
C	3.16700000	-0.90181600	-0.20476300
O	3.04169300	-1.29251300	0.92644200
O	2.66080600	-1.41976700	-1.29960700
H	2.09375600	-2.22263300	-1.10362600
C	-0.26339700	-0.60050800	3.35312000
H	-1.16722000	-0.50222100	2.74001600
H	0.27417300	-1.50738200	3.04955600
C	0.67211600	3.32875100	0.28631800
C	-0.00734600	1.93117800	0.25844600
O	-1.19187800	1.80232900	0.09259700
O	0.88884400	0.98999100	0.43272800
H	0.46641200	0.08322500	0.42338400
C	-4.14569700	0.97817500	-0.52831900
C	-3.33830600	-0.30097000	-0.17199600
O	-3.25297400	-0.68531800	0.96495200
O	-2.88195700	-0.87906900	-1.25898900
H	-2.42869800	-1.74687400	-1.05780300

Mn	-0.26695300	-2.94324100	0.03313400
H	0.38390100	0.27128000	3.19482600
H	-0.53693300	-0.66773700	4.41367800
F	3.48415300	1.11023500	-1.48389700
F	4.25120100	1.08190100	0.54333000
F	5.24031900	-0.07396700	-1.00499300
F	-0.23289900	4.30019600	0.16485400
F	1.55202600	3.44367300	-0.72250500
F	1.33652800	3.51359100	1.43894200
F	-3.64439300	1.64329700	-1.57324700
F	-4.21669200	1.80690000	0.51315800
F	-5.40831600	0.61001100	-0.84791600

INT2′(3TFA)

O	-1.95598100	-3.20157400	-0.66015800
O	0.77020200	-3.50534700	-0.72198700
O	-0.36050800	-1.19285100	-0.19059700
O	-0.49903800	-3.01897500	1.65139700
C	4.10654300	-0.02847800	-0.36672700
C	3.08350500	-1.14118900	-0.00247100
O	2.74451900	-1.32805400	1.13865600
O	2.72194800	-1.80377400	-1.07216400
H	2.03384700	-2.51232600	-0.86795900
C	-0.15826600	-0.31543400	2.82199000
H	-0.97983700	0.13357300	2.26730400
H	-0.39351200	-2.13996300	2.09369400
C	1.06756200	3.30912500	0.10564400
C	0.18493500	2.03105500	0.04073400
O	-1.01141900	2.07947400	0.17750100
O	0.93269600	0.97828600	-0.16292300
H	0.38585800	0.12210700	-0.17613500
C	-4.18992900	1.10591200	-0.37379100
C	-3.50789300	-0.23095200	0.03130500
O	-3.24970500	-0.48272500	1.18021200
O	-3.33813700	-0.98899000	-1.02393300
H	-2.87996900	-1.85560400	-0.80312100
Mn	-0.51788100	-2.80057300	-0.08085400
H	0.86178800	-0.24228300	2.44893000
H	-0.33473500	-0.69711000	3.82662800
F	3.78417000	0.61043000	-1.49762500
F	4.20004700	0.87098300	0.61362100
F	5.32525700	-0.58274400	-0.54049600
F	0.31749700	4.40455800	0.23672100
F	1.80921100	3.43890600	-1.00717900
F	1.90576500	3.24715000	1.15562500
F	-3.62781700	1.65505300	-1.45760900
F	-4.14699500	1.98924600	0.62225200
F	-5.48955500	0.87107800	-0.66265700

INT3′(3TFA)

O	-2.33908600	-2.40132900	0.17930000
O	-0.03511400	-1.81280000	-1.22398300
O	-0.69352100	-0.23008200	0.88089200
O	0.14760700	-2.80703800	1.36592900
C	4.58762300	-1.06331200	-0.44512400
C	3.08868300	-1.42525600	-0.24491900

O	2.66544400	-1.65965400	0.86853800
O	2.46257600	-1.46459800	-1.37741800
H	1.44550600	-1.63670200	-1.28506400
C	-1.02079700	-0.00249300	2.25050400
H	-0.78573200	1.04700000	2.47185900
H	1.06423100	-2.45298800	1.35678900
C	2.70779100	2.94224400	-0.05386700
C	1.40104200	2.28862500	0.47963000
O	0.68081700	2.86839700	1.25702800
O	1.26190800	1.09207000	-0.01550000
H	0.43555400	0.59401000	0.35124100
C	-5.73641100	0.84227400	-0.58689200
C	-4.63397000	-0.02862200	0.08197200
O	-4.28355600	0.16901500	1.21944600
O	-4.20738000	-0.93442500	-0.75501000
H	-3.46268600	-1.51493800	-0.35998000
Mn	-0.80859500	-1.89388300	0.20655000
H	-0.42829600	-0.65993600	2.90318900
H	-2.09110800	-0.18067700	2.41230600
F	4.75077300	-0.07829800	-1.33634600
F	5.14773800	-0.68631900	0.70592700
F	5.25184800	-2.14598900	-0.89754400
F	2.81239200	4.21182200	0.34436200
F	2.75244400	2.91988300	-1.39574000
F	3.78066900	2.27108700	0.40645500
F	-5.26811900	1.44100800	-1.69566000
F	-6.17160600	1.79099500	0.24456600
F	-6.78990500	0.08404400	-0.94220800

TS1′(3TFA)

O	-2.01108800	-3.16784400	-0.61550400
O	0.69853500	-3.50469600	-0.66122800
O	-0.39689700	-1.16381600	-0.18281300
O	-0.56489200	-2.92860900	1.65323900
C	4.10003900	-0.08177800	-0.45355100
C	3.07447000	-1.17682400	-0.04583300
O	2.78345800	-1.36055100	1.10878100
O	2.65404900	-1.82962700	-1.10016400
H	1.96363300	-2.52706600	-0.86744000
C	-0.26129900	-0.67108500	2.75832200
H	-1.05552100	-0.05030300	2.34044100
H	-0.42351300	-1.83832300	2.17740900
C	1.16200900	3.29107300	0.20553400
C	0.23944300	2.04082100	0.14660700
O	-0.95230400	2.12507300	0.30565300
O	0.95101300	0.96891800	-0.08318900
H	0.37904300	0.12848800	-0.11082300
C	-4.16408300	1.17346100	-0.45001000
C	-3.54407200	-0.18274800	-0.01044700
O	-3.33647900	-0.43410800	1.14878000
O	-3.35575800	-0.95139200	-1.05458300
H	-2.91853200	-1.82403200	-0.81313100
Mn	-0.57545900	-2.76698200	-0.02724400
H	0.75785400	-0.39272300	2.48259500
H	-0.39839000	-0.97238000	3.80070700
F	3.72681100	0.58149000	-1.55460100

F	4.27084000	0.80033400	0.53211700
F	5.29379600	-0.65949200	-0.70644300
F	0.45286300	4.40195800	0.41251700
F	1.84388000	3.43713700	-0.94352800
F	2.05519200	3.17225800	1.20355000
F	-3.51130500	1.71352800	-1.48704300
F	-4.16584000	2.04914200	0.55405100
F	-5.44559800	0.97770900	-0.83108200

TS2′(3TFA)

O	-2.17074400	-2.62077800	-1.38805800
O	0.52384400	-2.34699300	-1.75615500
O	-0.73830700	-1.07638500	0.16851200
O	-0.41125900	-3.60846300	0.49075300
C	4.33920500	-0.23408300	0.35719700
C	3.10379200	-1.14204000	0.09949100
O	2.74930900	-1.93267300	0.93757900
O	2.61962200	-0.96338100	-1.10263700
H	1.83511900	-1.56977100	-1.29894900
C	-0.19962300	-1.58643400	2.78972300
H	0.86835000	-1.72000800	2.62715700
H	-0.51996700	-3.20852100	1.38119300
C	1.24428800	3.21108500	-0.43400600
C	0.86417100	1.78565500	0.06031800
O	1.53079400	1.25963200	0.91858000
O	-0.17500300	1.30610400	-0.56373400
H	-0.39514000	0.35841100	-0.26113300
C	-4.41167600	1.22045900	0.38541300
C	-3.88755400	-0.23385400	0.21752100
O	-3.83609000	-0.99785600	1.14679400
O	-3.53841800	-0.43968800	-1.02785500
H	-3.10266600	-1.33961700	-1.15384800
Mn	-0.71801000	-2.41487200	-0.74610000
H	-0.76267200	-2.31481300	3.37089700
H	-0.62881300	-0.60042300	2.63968100
F	4.35551400	0.86816300	-0.39782200
F	4.40559100	0.12913700	1.64048800
F	5.45683200	-0.94101500	0.07336500
F	1.45545000	4.01931000	0.61590100
F	0.30658900	3.77098400	-1.20593300
F	2.38505100	3.14952500	-1.14309300
F	-3.44253400	2.10614500	0.09747200
F	-4.81855700	1.44152300	1.63673800
F	-5.44722000	1.45685600	-0.43896900

TS3′(3TFA)

O	-2.57704100	-2.51997300	0.67394200
O	-0.39905500	-1.76691500	-0.95567600
O	-0.40681800	-0.94473300	1.77307600
O	0.07533000	-3.15642500	1.45596300
C	4.26124500	-0.80885800	-1.26347300
C	2.84198600	-1.07372400	-0.68339500
O	2.65047700	-1.07896800	0.50872100
O	1.99142300	-1.28791500	-1.64644100
H	1.03667100	-1.48230300	-1.31381800
C	-1.31455400	-0.49931500	2.80571600

H	-0.73205900	0.10018500	3.51478500
H	0.14298600	-1.88338000	2.02143400
C	2.26688500	2.83664300	0.51129200
C	1.46088700	1.76666900	1.29839400
O	1.58983000	1.62120500	2.48771100
O	0.68507800	1.09806200	0.48355800
H	0.26186400	0.32508500	0.95707500
C	-4.88614800	1.22563200	-1.06520000
C	-3.84913600	0.31578800	-0.34573400
O	-2.86692100	0.78482100	0.17954500
O	-4.21776200	-0.93127400	-0.40736000
H	-3.53522800	-1.56687300	0.04348600
Mn	-0.97273600	-2.28696300	0.47256900
H	-1.75738700	-1.36797500	3.30554900
H	-2.08976600	0.10624100	2.33031300
F	4.23505300	0.11008700	-2.24156500
F	5.09731800	-0.38156800	-0.31450400
F	4.76745400	-1.94552500	-1.78170400
F	3.00258100	3.58499400	1.33408700
F	1.44988800	3.64892200	-0.17842000
F	3.09495300	2.24021500	-0.36638800
F	-5.04021800	0.85906300	-2.34916600
F	-4.50634200	2.50460800	-1.04153400
F	-6.08868700	1.13731800	-0.46557900

[MnO_4/4TFA]$^-$

Mn	-0.00291900	-2.72103900	0.00110600
O	-0.10781200	-1.80130100	1.29359900
O	1.30166700	-3.63274600	0.11948700
C	-2.03417000	2.63562000	1.20094100
C	-1.54163300	1.20981100	0.82921300
O	-1.04382200	0.60937600	1.87824200
H	-0.69318300	-0.29286800	1.63981800
O	-1.62288300	0.78992500	-0.29786700
F	-0.98533400	3.41586700	1.51942200
F	-2.86533400	2.60692500	2.25358300
F	-2.67476100	3.19848800	0.17651300
O	-1.30632100	-3.63400400	-0.12017600
O	0.10045000	-1.79720200	-1.28847500
O	-3.36800300	-2.15775400	-0.96305200
H	-2.68238700	-2.79276400	-0.61789300
C	-3.74235500	-1.31976600	-0.02490800
O	-3.42668400	-1.32115500	1.13672300
C	-4.74897600	-0.27683100	-0.58612400
F	-4.81424100	0.78983200	0.21484700
F	-5.97739200	-0.83041000	-0.64319700
F	-4.42677100	0.13557600	-1.81574900
O	1.04473900	0.60927900	-1.87694400
H	0.69245600	-0.29217100	-1.63799000
C	1.54339300	1.20920500	-0.82807600
O	1.62353100	0.78954700	0.29919800
C	2.03919700	2.63373200	-1.20035200
F	2.87274000	2.60222900	-2.25104100
F	2.67834000	3.19671800	-0.17508100
F	0.99248600	3.41539600	-1.52224900
H	2.67807400	-2.79350400	0.61664800

O	3.36498700	-2.15968300	0.96154600
C	3.73991800	-1.32204400	0.02341600
C	4.74921300	-0.28135400	0.58398400
O	3.42286200	-1.32220300	-1.13786000
F	4.42832800	0.13211300	1.81364700
F	4.81659000	0.78501200	-0.21723700
F	5.97632500	-0.83770200	0.64074600

[MnO_3/4TFA]$^-$

Mn	1.85307900	-1.27794200	1.83583400
O	1.12156100	-2.48100800	1.01723500
O	3.10166900	-1.57422400	2.74174700
C	-2.85679400	-1.64555100	-1.36545900
C	-1.38114300	-1.59988300	-0.87821300
O	-1.08705000	-2.57209400	-0.09311900
H	-0.11809500	-2.51940600	0.32422900
O	-0.65871800	-0.71651100	-1.31093500
F	-3.67591500	-2.22096500	-0.48240600
F	-2.91253100	-2.36139300	-2.50887400
F	-3.31138800	-0.41720700	-1.62850100
O	1.20835800	0.19687000	1.74620300
O	1.92463000	-0.32597400	-1.38515500
H	0.93123000	-0.45765800	-1.32237700
C	2.26926800	0.93394100	-1.29059300
O	1.55503200	1.90024700	-1.21668000
C	3.81869300	1.06075900	-1.28973000
F	4.19519500	2.33537600	-1.17698000
F	4.33494600	0.57194900	-2.43277000
F	4.35566700	0.37265700	-0.26866700
O	-0.73268500	1.73556700	1.17675400
H	0.02584300	1.08557500	1.39623400
C	-1.89633500	1.15652700	1.12135000
O	-2.17042600	-0.00273800	1.32533000
C	-2.99549000	2.18146500	0.72013500
F	-3.01646700	3.22298100	1.57113000
F	-4.20464700	1.61643500	0.72839700
F	-2.76642700	2.66187800	-0.51354400

INT1(4TFA)

Mn	-0.01593400	-2.44895800	-0.34137400
O	0.26029200	-1.44874200	-1.54615200
O	-1.26990900	-3.37141200	-0.69235200
C	2.03987600	-1.87616500	3.45368300
H	2.43265400	-2.89267400	3.58486100
H	1.56425200	-1.53921800	4.38353700
H	2.86190600	-1.20029300	3.18900500
H	1.30017400	-1.87381400	2.64417200
C	2.20082700	2.88647800	-0.56327500
C	1.74274200	1.40455100	-0.47056400
O	1.07396600	1.07032000	-1.54633000
H	0.80035300	0.11069100	-1.52974900
O	2.00109000	0.71873000	0.48488400
F	1.14216300	3.70171600	-0.69849600
F	3.00408900	3.06802900	-1.62432200
F	2.86854300	3.24518200	0.53295500
O	1.27085500	-3.35770000	-0.08613300

O	-0.32243100	-1.60024400	0.96797600
O	3.56926600	-2.15737700	0.48740000
H	2.76512300	-2.67705000	0.21051100
C	3.89384600	-1.26587000	-0.41633800
O	3.42800800	-1.11910300	-1.51712500
C	5.06578500	-0.37424800	0.08204600
F	5.06643700	0.79853700	-0.55854400
F	6.23635000	-0.99117500	-0.17879900
F	5.01107600	-0.13670200	1.39632000
O	-1.20943000	0.85853100	1.33109200
H	-0.89107100	-0.07513200	1.17564000
C	-1.94722900	1.29172600	0.33952600
O	-2.21512300	0.72421300	-0.68877200
C	-2.48106000	2.71744100	0.65119800
F	-3.23894800	2.70716400	1.75991000
F	-3.22167000	3.17632800	-0.35745200
F	-1.46369800	3.57105600	0.85081300
H	-2.78471000	-2.69039600	-0.85588000
O	-3.61410800	-2.16507900	-1.02930300
C	-3.95103600	-1.45665900	0.02074900
C	-5.18975900	-0.56611900	-0.27822600
O	-3.45100000	-1.46939900	1.11627600
F	-5.24223400	-0.15702400	-1.54888100
F	-5.19086400	0.51199700	0.51238300
F	-6.31191800	-1.26921000	-0.02280100

INT2(4TFA)

Mn	-0.03201600	-2.42341300	-0.02287000
O	0.13018600	-1.47913100	-1.29370100
O	-1.24562200	-3.45485200	-0.04672400
C	2.02221300	-1.53443500	3.24162900
H	2.27324300	-2.58956300	3.15010300
H	1.41830600	-1.19900400	4.08359500
H	2.52363400	-0.80559100	2.60754800
H	0.52263700	-1.47080500	2.02281400
C	2.16311900	2.84110300	-0.43816500
C	1.77591900	1.34098000	-0.31536200
O	1.02810200	0.98308400	-1.32430300
H	0.76934800	0.01283900	-1.29111500
O	2.15322000	0.66758400	0.61100500
F	1.06478300	3.61352700	-0.47372600
F	2.86249500	3.05937000	-1.56395800
F	2.91033300	3.22492000	0.59773400
O	1.37357800	-3.16332100	0.32143500
O	-0.22544200	-1.36061900	1.38545200
O	3.68906500	-2.06030800	0.43663900
H	2.79858500	-2.52905400	0.30883200
C	3.95484500	-1.24104000	-0.54393100
O	3.37585000	-1.11631300	-1.59463000
C	5.21888300	-0.38903600	-0.23498300
F	5.18270300	0.76535600	-0.90909200
F	6.32221500	-1.06142000	-0.62150500
F	5.34617100	-0.10799400	1.06731200
O	-1.26522800	0.98948200	1.44513500
H	-0.87869200	0.05301000	1.37099600
C	-1.99725600	1.31938700	0.41515200

O	-2.20562200	0.68245500	-0.58715600
C	-2.63516600	2.72029300	0.63090400
F	-3.49493600	2.68770300	1.66494200
F	-3.30451700	3.11319400	-0.45339400
F	-1.69728300	3.64257600	0.90252700
H	-2.67493300	-2.80852000	-0.63000900
O	-3.46403200	-2.30441800	-0.97739400
C	-3.95925200	-1.51315700	-0.05673700
C	-5.13351600	-0.66755100	-0.62440600
O	-3.63887500	-1.43066000	1.10140600
F	-4.94316100	-0.30090000	-1.89511900
F	-5.31993900	0.43251600	0.11008100
F	-6.26796300	-1.39786200	-0.57168200

INT3(4TFA)

Mn	0.03503100	-0.93887200	0.79075600
O	0.50176000	-0.78125400	-0.74053200
O	-1.27906700	-1.79363300	1.12847500
C	1.73826300	-0.92575400	3.04635000
H	2.61795300	-1.45651600	3.43529400
H	0.88795100	-1.09437900	3.71961100
H	1.95859700	0.14820100	2.99400700
H	0.59102700	1.27457400	1.21509200
C	3.99160600	2.49436900	-0.81613100
C	2.72272200	1.68090600	-0.43869500
O	2.48256600	0.74460700	-1.30607300
H	1.65834100	0.18259000	-1.08585500
O	2.07471900	1.99436800	0.53720600
F	3.63468000	3.48700800	-1.65699700
F	4.91427100	1.74782900	-1.43061400
F	4.54232000	3.04745000	0.26479800
O	1.46172900	-1.45096500	1.75176000
O	-0.18569300	0.72222500	1.45901900
O	3.48499300	-2.13453300	0.38177300
H	2.67152700	-1.86152500	0.94729000
C	4.41114800	-1.21784800	0.39094700
O	4.41616800	-0.17094800	0.99457800
C	5.59234500	-1.61986600	-0.53674900
F	6.60111200	-0.75386000	-0.43231700
F	5.18983300	-1.64346900	-1.81906600
F	6.05692100	-2.84253600	-0.22695500
O	-2.47956200	1.78662400	1.36202100
H	-1.53904900	1.36449800	1.35951900
C	-3.11346900	1.58382800	0.24251700
O	-2.72609000	1.00382800	-0.74400000
C	-4.51333900	2.26158200	0.26094000
F	-5.13514100	2.13323400	1.43900300
F	-5.30438500	1.75561600	-0.68945600
F	-4.36930300	3.58287600	0.01606500
H	-2.51131400	-2.01636000	0.16521700
O	-3.28069600	-2.16343100	-0.47428400
C	-4.36565200	-1.55153300	-0.08243200
C	-5.49443400	-1.72783300	-1.13707900
O	-4.54437500	-0.92134500	0.93049800
F	-5.14040100	-1.17805600	-2.30970600
F	-6.62567900	-1.15042600	-0.72945400

F	-5.74617800	-3.03241300	-1.35203300

TS1(4TFA)

Mn	-0.05361600	-2.41520500	-0.04370300
O	0.15065500	-1.47137900	-1.30693600
O	-1.24614700	-3.46825400	-0.15745600
C	1.54824200	-1.64289600	3.05291200
H	1.66256400	-2.70957700	3.25335800
H	1.08317900	-1.06478800	3.85637200
H	2.39837700	-1.16427200	2.56439800
H	0.61999000	-1.57025600	2.15686800
C	2.21483100	2.82472100	-0.44560100
C	1.78894400	1.33516500	-0.32425100
O	1.07106200	0.98396200	-1.35802300
H	0.79560000	0.01898000	-1.32324800
O	2.11168900	0.66262800	0.62288800
F	1.13445400	3.62166500	-0.50153000
F	2.93778500	3.02449800	-1.55942900
F	2.95241000	3.19430800	0.60223100
O	1.33663600	-3.16350000	0.35023100
O	-0.29769300	-1.42879100	1.32938700
O	3.65202900	-2.08014400	0.48739000
H	2.75908000	-2.54543100	0.35081900
C	3.93611800	-1.26769300	-0.49353600
O	3.37437700	-1.14686100	-1.55395600
C	5.19724400	-0.41630500	-0.17119400
F	5.16774700	0.73773900	-0.84679300
F	6.30460200	-1.08866100	-0.54553900
F	5.31063100	-0.13378200	1.13203300
O	-1.23041000	0.99994300	1.43624200
H	-0.87281700	0.06206900	1.35237400
C	-1.95912100	1.34894300	0.40678400
O	-2.17887600	0.72000200	-0.59675600
C	-2.56895100	2.76054100	0.63206900
F	-3.42446700	2.73872500	1.66935700
F	-3.23470900	3.16913800	-0.44806700
F	-1.61207600	3.66253900	0.90339100
H	-2.68952700	-2.81060400	-0.67715700
O	-3.47985100	-2.29343200	-1.00341800
C	-3.94335200	-1.49893400	-0.06909700
C	-5.11282500	-0.62937400	-0.61041300
O	-3.59877200	-1.42739100	1.08272200
F	-4.93503600	-0.25339400	-1.88036000
F	-5.26987500	0.46665200	0.13706600
F	-6.25817900	-1.34112400	-0.54744600

TS2(4TFA)

Mn	0.03725600	-2.24414700	0.11621700
O	0.25134400	-1.35719200	-1.18445900
O	-1.08025200	-3.37771300	0.08354100
C	2.16886800	-1.85007700	3.08574900
H	2.77963800	-2.73032300	2.90953500
H	1.36196400	-1.91273900	3.81540300
H	2.50973100	-0.88122700	2.72552600
H	0.46114200	-1.19269800	2.08517500
C	2.05546000	2.97681600	-0.00125500

C	1.72202100	1.45904300	0.00157700
O	1.01401500	1.14627900	-1.05117700
H	0.82565600	0.16070700	-1.10595900
O	2.11674400	0.73367500	0.87959300
F	0.96615800	3.72148500	-0.23815400
F	2.96043600	3.24423800	-0.96105900
F	2.57158500	3.35120900	1.17098100
O	1.46872700	-2.81068400	0.67565500
O	-0.29903300	-1.13624200	1.46963200
O	3.84553800	-1.91197700	0.32848600
H	2.88493700	-2.24107300	0.37527100
C	4.06645000	-1.11242500	-0.67899700
O	3.32174600	-0.80950200	-1.57729400
C	5.50173700	-0.52053500	-0.58777600
F	5.80315500	0.17905300	-1.68327000
F	6.42287500	-1.48852400	-0.44342200
F	5.59850100	0.30233900	0.47243800
O	-1.45049800	1.14086600	1.30762200
H	-1.01290400	0.22046700	1.33867100
C	-2.17019600	1.31921200	0.23313600
O	-2.32007200	0.56760400	-0.69823000
C	-2.88732200	2.69745300	0.28123900
F	-3.75778000	2.73607500	1.30635900
F	-3.56370500	2.92445300	-0.84564600
F	-2.00582000	3.69659400	0.45045000
H	-2.54279300	-2.88354300	-0.54038600
O	-3.36998300	-2.46158000	-0.90988500
C	-3.93475500	-1.68084400	-0.02140200
C	-5.16846300	-0.95093400	-0.62239700
O	-3.63288600	-1.53212400	1.13508600
F	-5.02689900	-0.66913100	-1.92063200
F	-5.40709700	0.18840700	0.03411200
F	-6.25526200	-1.74102300	-0.48843200

TS3(4TFA)

Mn	-0.05399200	-2.20947100	-0.35807700
O	0.51275700	-1.31556500	-1.55375800
O	-1.28794300	-3.19904700	-0.61454800
C	1.20440200	-4.37989600	1.24462800
H	1.95448600	-4.55097000	2.02580400
H	1.41437200	-5.00966200	0.37499400
H	0.19897100	-4.58657900	1.62911000
H	0.78305700	-2.24871100	1.45738700
C	2.16191500	3.07255500	-0.39712100
C	1.89707400	1.54130600	-0.35126700
O	1.14555300	1.18255600	-1.35615600
H	0.96243100	0.18741300	-1.38351300
O	2.37556600	0.85065300	0.51377300
F	1.01846900	3.76593500	-0.49947300
F	2.92794400	3.37631000	-1.46229700
F	2.80144100	3.47919400	0.70098100
O	1.29601200	-2.99961500	0.83198400
O	-0.20181100	-1.32865200	1.12706400
O	3.73796400	-1.88187900	0.87276000
H	2.89371500	-2.37810500	0.70862600
C	4.13325800	-1.23821200	-0.20120700

O	3.69453900	-1.32499100	-1.31803300
C	5.36119900	-0.33594300	0.10278600
F	5.38639600	0.71278200	-0.72417200
F	6.48986900	-1.04982600	-0.09769000
F	5.38255600	0.11621700	1.35949300
O	-1.17556200	0.90532700	1.35958000
H	-0.77214200	-0.09161200	1.22750500
C	-1.96807300	1.26599200	0.40503300
O	-2.26347400	0.66336400	-0.60530100
C	-2.58816500	2.66456700	0.69223200
F	-3.32875200	3.09110800	-0.33508200
F	-1.63510700	3.58439800	0.92482900
F	-3.38126800	2.61408700	1.78016100
H	-2.79360200	-2.62085200	-0.78897900
O	-3.64009900	-2.12770700	-1.00871300
C	-4.07993100	-1.44501500	0.01745300
C	-5.28658800	-0.54908700	-0.38100400
O	-3.69883100	-1.48568000	1.15987500
F	-5.22655200	-0.11732400	-1.64418300
F	-5.36927600	0.51453000	0.42411700
F	-6.42787800	-1.25984000	-0.24406300

$[MnO_4/Sc(OTf)_3]^-$

Sc	-0.33995700	0.12984800	-0.18184100
O	-0.10372900	1.61004800	-1.78857700
O	-1.57248900	-1.16919500	1.08026600
O	1.09448800	0.24722100	1.24932900
S	-2.84208000	-1.07711300	0.24522200
S	2.12519500	-0.66288600	1.94450000
S	-0.57922500	2.81879700	-0.99427700
O	-2.43959500	-0.16558400	-0.89812400
O	-3.54846700	-2.30946500	-0.06698800
O	1.81349000	-2.08733600	1.78572500
O	2.47243500	-0.14750800	3.27324300
O	-0.91902000	2.24390100	0.36451400
O	-1.53663600	3.71291800	-1.62892600
C	0.98888700	3.82487400	-0.70482700
C	-4.01482000	-0.03917100	1.29607300
C	3.63426400	-0.33647700	0.86410200
F	0.69675800	4.87125500	0.05844400
F	1.89578400	3.06804700	-0.10022900
F	1.45989300	4.24122900	-1.87469500
F	3.37568000	-0.66465500	-0.39894300
F	4.65457100	-1.06874900	1.30842200
F	3.96463400	0.95355900	0.91999500
F	-4.33226800	-0.72063100	2.39038400
F	-3.42372200	1.09932300	1.63151300
F	-5.11177700	0.21487000	0.59194300
Mn	0.58979300	-2.90108700	-1.61117000
O	0.46932000	-1.25556500	-1.30975700
O	0.12346800	-3.17333700	-3.08481200
O	-0.32774700	-3.67559800	-0.60552300
O	2.08273900	-3.34349700	-1.43322000

$[MnO_3/Sc(OTf)_3]^-$

Sc	-0.47036300	-0.17366800	-0.45231700

O	-0.57235000	1.62373400	-1.71783900
O	-1.58543900	-1.59451000	0.85427000
O	0.90440300	-0.04539900	1.19554900
S	-2.79082700	-1.73158300	-0.05650000
S	2.22915700	-0.69847300	1.47299400
S	-1.20221900	2.57139700	-0.70550400
O	-2.48777000	-0.78721700	-1.20406500
O	-3.25563200	-3.07394900	-0.37938000
O	2.49908300	-1.92475200	0.61511700
O	2.53035700	-0.92766000	2.87978900
O	-1.35159800	1.74825300	0.54738700
O	-2.33546900	3.37136100	-1.15490600
C	0.18054300	3.78898000	-0.31815700
C	-4.19997400	-0.91313000	0.89096100
C	3.48014700	0.56283300	0.83670900
F	-0.20795700	4.59334500	0.66588300
F	1.26775000	3.12198500	0.05565900
F	0.45238700	4.50945500	-1.40099200
F	3.20406200	0.86690000	-0.42464800
F	4.69726100	0.04361000	0.91914800
F	3.40537700	1.65460000	1.58808000
F	-4.43585800	-1.61319300	1.99646000
F	-3.87202900	0.32990300	1.21088000
F	-5.28761100	-0.90742300	0.12684700
Mn	2.00645000	-2.44814600	-1.18334400
O	0.72747900	-1.23150600	-1.38714200
O	3.26278000	-2.17114900	-2.10209200
O	1.43463800	-3.91664600	-1.07000400

INT1[Sc(OTf)$_3$]

Sc	0.29511100	0.11638600	0.05118000
O	-0.08822800	1.54462300	1.65951000
O	1.56506600	-0.93484200	-1.39064800
O	-1.25393300	0.29748800	-1.24819500
S	2.84056100	-0.91054900	-0.55803900
S	-2.31958300	-0.61288600	-1.89089300
S	0.41595100	2.78856700	0.93812300
O	2.43097600	-0.14827000	0.68607500
O	3.57010800	-2.15840300	-0.39388400
O	-1.94883500	-2.03106100	-1.83467700
O	-2.80691200	-0.04587900	-3.15267200
O	0.84479800	2.26619800	-0.41484000
O	1.32318600	3.66669500	1.66299300
C	-1.14547200	3.79185000	0.60544600
C	3.99068100	0.25721100	-1.49170900
C	-3.72734800	-0.39305000	-0.65691500
F	-0.82982000	4.84574500	-0.13841000
F	-2.03208500	3.04110900	-0.03250100
F	-1.65186900	4.19762800	1.76452500
F	-3.32883800	-0.74710600	0.56193100
F	-4.75265200	-1.15975200	-1.02450300
F	-4.11934900	0.88035900	-0.63437500
F	4.31503800	-0.29616400	-2.65452000
F	3.38350700	1.41595200	-1.70003100
F	5.08662700	0.44803700	-0.76571500
Mn	-0.42751800	-3.05948700	1.22765200

O	-0.35860500	-1.38639800	1.13100800
O	0.22825700	-3.49763800	2.58637100
C	1.46175100	-0.48124500	3.92909800
H	1.78217700	-0.62468900	4.96859300
H	0.75648800	0.35539900	3.86542800
H	2.33013400	-0.26509900	3.29567400
H	0.97413400	-1.39347900	3.56388400
O	0.36425200	-3.67869000	0.02750300
O	-1.92711500	-3.51283000	1.18272200

INT2[Sc(OTf)$_3$]

Sc	0.29876900	0.08415700	0.01848400
O	0.06061000	1.51089000	1.67484100
O	1.57990400	-1.00009900	-1.39485100
O	-1.20002900	0.29913000	-1.34854700
S	2.83826900	-1.00552900	-0.53932100
S	-2.33021300	-0.57061200	-1.92783900
S	0.57706100	2.74534100	0.94820800
O	2.43363700	-0.22437600	0.69392200
O	3.53321200	-2.27120100	-0.35576500
O	-2.09197700	-2.00587900	-1.73496500
O	-2.74916300	-0.08614200	-3.24791500
O	0.91154100	2.24168100	-0.43597300
O	1.55447400	3.57332400	1.64224100
C	-0.95732400	3.81535100	0.71594100
C	4.03647000	0.12456100	-1.45731300
C	-3.73316400	-0.11898300	-0.75370600
F	-0.63666800	4.87984100	-0.01100100
F	-1.89952400	3.11715100	0.09538800
F	-1.40062300	4.20490800	1.90659200
F	-3.38350100	-0.38367500	0.50318000
F	-4.81416100	-0.83141200	-1.06759600
F	-4.01932700	1.17833400	-0.86166400
F	4.37021000	-0.44426700	-2.61030900
F	3.46491800	1.29799900	-1.68549600
F	5.12324100	0.29248800	-0.71111800
Mn	-0.65457200	-3.03304600	1.19473600
O	-0.41741700	-1.34995000	1.07993200
O	0.13987100	-3.29039900	2.73140000
C	1.23384700	-0.78926100	3.79282300
H	1.40164000	-1.30352400	4.73797400
H	0.36866100	-0.14000000	3.67589300
H	2.02773600	-0.74782800	3.04913600
H	0.49466800	-2.42885500	3.07347500
O	0.13724300	-3.78202900	0.07282200
O	-2.17746900	-3.36750600	1.33560100

INT3[Sc(OTf)$_3$]

Sc	0.34344500	-0.23881400	-0.56962900
O	-0.67903100	-1.09525800	-2.30952900
O	1.59416500	-0.39135100	1.24994600
O	-0.93082100	0.91751400	0.52053700
S	2.56391800	-1.42064900	0.69677100
S	-1.27475900	1.23656000	1.98274900
S	-1.42215700	-2.21561400	-1.59002900
O	2.02066800	-1.71302800	-0.68912000

O	3.99005000	-1.15862600	0.82915000
O	-0.36824300	2.23675900	2.55934200
O	-1.59849900	0.03639200	2.76298300
O	-1.01154900	-2.06582800	-0.14778500
O	-1.38108300	-3.53993100	-2.19694300
C	-3.22395500	-1.66666500	-1.64229200
C	2.22667300	-2.98333700	1.69719600
C	-2.90621900	2.13330100	1.71293500
F	-3.95654700	-2.51146700	-0.92525000
F	-3.33253500	-0.44315900	-1.13934500
F	-3.64606300	-1.66948600	-2.90289200
F	-2.71865200	3.20541000	0.94200700
F	-3.38754400	2.52523600	2.89255800
F	-3.78905200	1.32639600	1.12824700
F	0.93442400	-3.26837800	1.67391000
F	2.91823000	-3.98712600	1.16585500
F	2.62137500	-2.78432400	2.95002500
Mn	2.33723300	2.41237900	-1.35772600
O	1.22687400	1.13950300	-1.58925300
O	3.28372000	2.78480100	-2.80286300
C	0.20484800	3.94802100	-0.59922600
H	-0.55470800	3.21114500	-0.90016600
H	-0.20788500	4.96148700	-0.70937500
H	0.45777100	3.77462600	0.45765200
H	2.98272000	3.61235000	-3.21042200
O	3.15919200	2.41555800	-0.03303800
O	1.34531600	3.86042000	-1.43366500

TS1[Sc(OTf)$_3$]

Sc	0.27577500	0.08098700	0.00817200
O	0.17456800	1.48517500	1.71660000
O	1.52132300	-0.99585200	-1.43929500
O	-1.20834600	0.35032100	-1.37368300
S	2.78807600	-1.05080000	-0.59795600
S	-2.33864600	-0.48783600	-1.99416900
S	0.66925300	2.71871900	0.97589600
O	2.41339200	-0.29175000	0.65753100
O	3.45523900	-2.33656200	-0.45449100
O	-2.11411900	-1.93125900	-1.85445100
O	-2.74356200	0.04829100	-3.29893400
O	0.91798400	2.22984500	-0.43174300
O	1.69456900	3.52668700	1.62332400
C	-0.86108700	3.80990300	0.83518800
C	4.00311300	0.07440700	-1.49967600
C	-3.74838900	-0.06627000	-0.81712900
F	-0.56564500	4.88274400	0.10970200
F	-1.83995100	3.13048400	0.24985000
F	-1.24351000	4.18539000	2.05136900
F	-3.41586100	-0.38445300	0.43220200
F	-4.83541900	-0.75141600	-1.16952500
F	-4.01699700	1.23829400	-0.87621600
F	4.30843200	-0.46903600	-2.67268200
F	3.45972800	1.26818500	-1.68677700
F	5.10295200	0.19292700	-0.76280800
Mn	-0.67939300	-3.01037700	1.28634600
O	-0.47084700	-1.33016800	1.06899000
O	0.13453800	-3.19315700	2.75721100

C	1.14249400	-1.06896800	3.67208600
H	1.41206900	-1.44013200	4.66438200
H	0.35005800	-0.31919400	3.64491600
H	1.97591900	-0.87901300	2.99297500
H	0.60094600	-2.14077900	3.17237700
O	0.06917600	-3.80264900	0.16367400
O	-2.19950700	-3.34342200	1.46975500

TS2[Sc(OTf)$_3$]

Sc	-0.44949200	-0.08928400	-0.14636700
O	-0.94305100	1.14643400	-1.89696500
O	-1.03185700	-1.63793200	1.30250000
O	0.39991500	1.04458800	1.33980100
S	-1.88174700	-2.46452200	0.34867500
S	1.70663100	1.00518000	2.14892500
S	-2.17735900	1.82602700	-1.31924200
O	-1.83654900	-1.67734800	-0.94394000
O	-1.63994100	-3.89919900	0.29237800
O	2.38161400	-0.29684700	2.07261800
O	1.54419400	1.64786800	3.45829100
O	-2.29774500	1.25184900	0.07187500
O	-3.36906200	1.87939000	-2.15602300
C	-1.63226900	3.61145100	-1.06034300
C	-3.64426700	-2.25808600	0.98664300
C	2.76310400	2.18866700	1.13359600
F	-2.59906900	4.27471700	-0.43524000
F	-0.52580800	3.63943600	-0.32816600
F	-1.39943500	4.17203300	-2.24263800
F	2.86717400	1.75246700	-0.11969400
F	3.97948700	2.26400700	1.67335200
F	2.21320900	3.40310200	1.12730900
F	-3.74160100	-2.83594700	2.17943300
F	-3.94282000	-0.97149500	1.08714400
F	-4.47925500	-2.84702300	0.13636000
Mn	2.36068000	-1.99459500	-0.80486900
O	1.13002300	-0.82561300	-0.95380700
O	2.26947200	-2.74358600	-2.39982500
C	5.47843300	-2.18656700	-2.78874500
H	5.47439600	-3.26625900	-2.93580000
H	6.08623400	-1.75331300	-1.99884800
H	4.92531900	-1.53998000	-3.46671000
H	3.09131500	-3.22609100	-2.59164000
O	2.03055000	-3.06843700	0.28163000
O	3.78090700	-1.33816000	-0.71765100

TS3[Sc(OTf)$_3$]

Sc	-0.46618200	-0.05411400	-0.17392100
O	-0.38183600	1.32159000	-1.90718600
O	-1.71835800	-1.15532500	1.26274800
O	0.90699000	0.36852800	1.29173800
S	-2.92789100	-1.33215100	0.35749300
S	2.17799000	-0.19416000	1.93921200
S	-1.04355100	2.51862700	-1.24049300
O	-2.54445800	-0.59343900	-0.90550500
O	-3.48773100	-2.67119800	0.23180600
O	2.61400200	-1.46391400	1.34203900

O	2.14163000	-0.07443600	3.40085700
O	-1.31579300	2.05804300	0.17064600
O	-2.10987800	3.19149400	-1.97164600
C	0.35136200	3.77278200	-1.07184000
C	-4.27082700	-0.27894700	1.15814800
C	3.43000500	1.08439400	1.35477500
F	-0.09107200	4.82980900	-0.39925000
F	1.36908700	3.22304900	-0.41921400
F	0.75117600	4.15031400	-2.28208800
F	3.44719300	1.12801200	0.02067300
F	4.64196100	0.74432800	1.79237800
F	3.11902600	2.28957500	1.82544100
F	-4.58848200	-0.80631400	2.33600200
F	-3.83454400	0.96057400	1.32635600
F	-5.34013300	-0.27494500	0.36851300
Mn	0.91270600	-3.11226200	-1.05453000
O	0.42355700	-1.46854300	-1.09516100
O	0.83659700	-3.88063700	-2.55477100
C	3.40068300	-1.84188500	-1.87111600
H	2.82156900	-1.21895600	-2.56653800
H	4.38297700	-2.07047300	-2.30552100
H	3.52294600	-1.31894500	-0.91913600
H	2.08090200	-3.57083600	-2.49789800
O	0.66492800	-3.96780700	0.22457000
O	2.73582400	-3.08592800	-1.63186400

INT1′[Sc(OTf)$_3$]

Mn	1.13160800	0.69641800	2.59351300
O	0.71749300	2.11660800	3.09400400
O	2.14707400	0.04080900	3.58296000
O	-0.17950300	-0.25425700	2.35942700
O	1.71563700	0.75008700	1.08188700
C	-2.64520800	1.87726600	2.31351700
H	-2.30891900	2.20793400	1.32484400
H	-3.61097100	2.34429000	2.54508400
H	-2.75504100	0.78740400	2.31251100
H	-1.90336200	2.17219100	3.06589400
Sc	0.10583300	-0.50785000	0.25857600
O	-0.69505700	1.12253000	-0.57571300
O	1.35624800	-0.82950400	-1.53410000
O	-1.50162000	-1.70656000	0.10153700
S	2.05224800	-2.08026800	-1.02003600
S	-2.95625700	-2.09356800	0.41839100
S	-0.80698100	2.29632400	-1.56116400
O	1.48555800	-2.24019500	0.38065200
O	2.07621800	-3.25047200	-1.88474400
O	-3.36159600	-1.67340100	1.76384200
O	-3.24334600	-3.46181400	-0.02356000
O	-1.92347100	3.17813700	-1.20914500
O	-0.64307800	1.86412200	-2.95235000
C	0.75722000	3.25095400	-1.12255700
C	3.85879600	-1.58529400	-0.78109400
C	-3.87565700	-0.96579200	-0.78067400
F	0.80474200	4.36478200	-1.85187400
F	0.74791600	3.57254600	0.16880900
F	1.83166200	2.51033800	-1.38515300

F	-3.67483100	0.30770300	-0.45925000
F	-5.17879000	-1.23621400	-0.71250100
F	-3.44819300	-1.17914900	-2.02333600
F	4.37569900	-1.29361600	-1.96900700
F	3.95117600	-0.53549200	0.01854500
F	4.50906800	-2.61409200	-0.24890200

INT2′[Sc(OTf)$_3$]

Mn	0.85424300	1.26286100	2.61095500
O	0.09329000	2.80017100	2.45021700
O	1.51062600	1.04021900	4.00637700
O	-0.44815100	0.24172400	2.39440700
O	1.68221500	0.82691500	1.27580500
C	-2.63033100	2.46640000	1.60103500
H	-2.35853500	2.82705700	0.60895200
H	-2.98155900	3.17295000	2.35232800
H	-2.77391300	1.39908700	1.75993300
H	-0.85117600	2.72104100	2.12486500
Sc	0.13420900	-0.49856900	0.53564300
O	-0.58550800	1.02862800	-0.57848700
O	1.31256600	-1.10844100	-1.27469000
O	-1.51555900	-1.68149000	0.36464500
S	2.01708900	-2.26807000	-0.60114800
S	-3.01662200	-1.81200600	0.65631500
S	-0.61450500	1.90150300	-1.83574600
O	1.49019400	-2.22663200	0.82459000
O	2.03168100	-3.55726600	-1.27806300
O	-3.46755200	-0.89762500	1.71407000
O	-3.42956600	-3.21860800	0.70995300
O	-1.62283900	2.96246600	-1.71100700
O	-0.55456600	1.11834800	-3.07362600
C	1.04985000	2.77164200	-1.68780100
C	3.82138300	-1.73267900	-0.47075900
C	-3.74223900	-1.13018200	-0.94384500
F	1.19219900	3.61929900	-2.70674700
F	1.10745000	3.45000900	-0.54369600
F	2.03840700	1.88094800	-1.71946600
F	-3.44629400	0.16132500	-1.06831400
F	-5.06750600	-1.27215300	-0.91148600
F	-3.25656900	-1.79554700	-1.98896800
F	4.34274800	-1.69283600	-1.69214700
F	3.90369300	-0.53566000	0.08958500
F	4.48017200	-2.62015200	0.26740600

INT3′[Sc(OTf)$_3$]

Mn	1.03741400	0.73524500	-2.59764000
O	2.10731100	-0.09905000	-3.69337500
O	0.15704500	2.06035500	-3.24608100
O	-0.17570000	-0.38311700	-2.26020600
O	1.52518600	0.90429300	-1.04361100
C	-1.22764400	2.31965700	-3.05849100
H	-1.79443300	1.37935100	-3.01984700
H	-1.56270600	2.93170100	-3.90678800
H	-1.37463600	2.86698000	-2.11759300
H	1.83529600	-1.01073200	-3.88833900
Sc	0.03175300	-0.38188000	-0.22120400

O	1.39378400	-1.81661800	0.22736200
O	0.25841400	0.55335200	1.80136100
O	-1.68080200	-1.51020000	0.00027400
S	-0.73288400	1.67814300	1.57132200
S	-3.07217200	-1.57720700	-0.64406800
S	2.59396500	-2.34098400	1.02243500
O	-1.19815700	1.47468400	0.14441200
O	-1.74389700	1.91129100	2.59507600
O	-3.40247000	-2.93867600	-1.08543100
O	-3.34023800	-0.45689100	-1.55622500
O	3.17035100	-3.53295100	0.38841100
O	2.34444400	-2.35507600	2.46856800
C	3.84880300	-0.96322700	0.73984200
C	0.30355400	3.25352700	1.53371500
C	-4.14354300	-1.26030000	0.86994800
F	4.98678200	-1.28101100	1.35821900
F	4.08711300	-0.81721200	-0.56189700
F	3.38961200	0.18334800	1.23599300
F	-3.92505700	-2.19438800	1.79500700
F	-5.42832700	-1.29653100	0.51130100
F	-3.86784200	-0.06424900	1.38412900
F	0.81718800	3.45794200	2.74290100
F	1.28047200	3.15259600	0.64601800
F	-0.48854400	4.27314200	1.20938300

TS1′[Sc(OTf)$_3$]

Mn	-0.92804500	-1.33648800	2.51846900
O	-0.18422800	-2.81747800	2.34320100
O	-1.64127700	-1.18173800	3.89769100
O	0.36599200	-0.28597000	2.38849000
O	-1.72442300	-0.87768700	1.17713300
C	2.28928400	-2.68364100	1.74012500
H	2.24208000	-2.99610400	0.69294300
H	2.71843900	-3.41396100	2.43196900
H	2.59375100	-1.64700100	1.89590500
H	1.06774500	-2.72764900	2.05499800
Sc	-0.14537000	0.48902300	0.53801800
O	0.63331300	-0.99625800	-0.59037900
O	-1.31020300	1.14436500	-1.26534800
O	1.51468300	1.67043000	0.47338600
S	-2.02484600	2.28256300	-0.56568300
S	3.01537800	1.68679800	0.80038200
S	0.71543300	-1.84018800	-1.86490000
O	-1.51532000	2.19801200	0.86459100
O	-2.03029100	3.59149100	-1.20390600
O	3.42184800	0.56270200	1.65457600
O	3.47251700	3.03869000	1.14059100
O	1.74515100	-2.87981700	-1.73850500
O	0.66746900	-1.03101600	-3.08684300
C	-0.93178100	-2.74980100	-1.78130100
C	-3.83188300	1.74685100	-0.47563600
C	3.74321400	1.31600400	-0.89780400
F	-1.02938200	-3.57365500	-2.82486100
F	-1.00429700	-3.45868700	-0.65693100
F	-1.93823000	-1.87935700	-1.81694900
F	3.41199900	0.08547300	-1.28103100

F	5.07145500	1.40712600	-0.82652100
F	3.29295300	2.19153900	-1.79344400
F	-4.33383900	1.73807200	-1.70577400
F	-3.92645000	0.53734300	0.05434100
F	-4.49958800	2.61863100	0.27312300

TS2′[Sc(OTf)$_3$]

Mn	-2.00987200	-1.06583600	1.80756400
O	-1.80593300	-2.78167800	2.05583000
O	-3.24449400	-0.58025500	2.63464600
O	-0.59230900	-0.38555100	2.34219500
O	-1.91169300	-0.64032200	0.24242300
H	-2.67782100	-3.21719300	2.09012200
Sc	0.03704700	0.31456000	0.47053200
O	0.85458100	-1.11623700	-0.69785800
O	-0.34607500	1.53001800	-1.35583600
O	1.82488600	0.98791800	1.19951200
S	-0.93254300	2.72527700	-0.62682600
S	3.11104300	0.39678100	1.80114900
S	1.11658200	-1.80813900	-2.03879600
O	-0.90895300	2.29618200	0.82934900
O	-0.42014600	4.04734200	-0.95871100
O	2.99299200	-1.04137900	2.07447300
O	3.67300100	1.27553000	2.83335400
O	1.86024800	-3.05904300	-1.85511700
O	1.54816700	-0.86929400	-3.08026500
C	-0.63302900	-2.31991000	-2.51564200
C	-2.75827200	2.75187100	-1.10357300
C	4.27274200	0.54774600	0.32561800
F	-0.59114400	-2.99768900	-3.66331200
F	-1.16159500	-3.09602700	-1.57094100
F	-1.39725900	-1.24124400	-2.67566600
F	3.83202900	-0.19258800	-0.68788100
F	5.48451200	0.12241100	0.68392000
F	4.35517700	1.81896500	-0.06432900
F	-2.85427300	2.98517000	-2.40808700
F	-3.32899600	1.59320000	-0.81314200
F	-3.35826300	3.72794500	-0.42968300
H	-4.04427500	-3.05211400	4.22719300
H	-4.93926700	-3.53742200	2.63662700
H	-5.36017700	-1.91913700	3.49839100
C	-4.75591000	-2.82034400	3.43678000

TS3′[Sc(OTf)$_3$]

Mn	1.11445500	1.29429500	-2.38676400
O	2.09284600	1.82433800	-3.64162400
O	0.80199600	3.15743100	-2.36820800
O	-0.31095300	0.46777900	-2.43248200
O	1.67714700	0.88806600	-0.89304100
C	1.04288900	3.94098100	-1.19403600
H	0.29068200	3.68257300	-0.44208400
H	0.93989400	4.99509300	-1.48098900
H	2.05024400	3.75614300	-0.79882800
H	1.63852400	2.94404900	-3.19340300
Sc	-0.10066600	-0.27127300	-0.44446900
O	0.98445600	-1.97631600	-0.46607900

O	0.11875300	-0.22821500	1.76106000
O	-1.96173500	-1.08921400	-0.57716500
S	-0.52787100	1.12875700	1.97336500
S	-3.36621000	-0.75161700	-1.10607300
S	1.99772500	-2.93834100	0.16958700
O	-0.88063100	1.57917100	0.56908400
O	-1.54508400	1.25001700	3.00771800
O	-3.85561300	-1.77689600	-2.03494500
O	-3.51609400	0.66336000	-1.46652200
O	2.43889900	-3.95146800	-0.79570200
O	1.59813000	-3.36256900	1.51555300
C	3.47827800	-1.79678600	0.41570000
C	0.88575800	2.25520700	2.51582500
C	-4.35121000	-0.98025700	0.48099000
F	4.46643700	-2.48989700	0.98221300
F	3.89450800	-1.32418000	-0.75674900
F	3.14857600	-0.78045300	1.20947700
F	-4.22649400	-2.22927600	0.92625500
F	-5.63813900	-0.73156500	0.23557600
F	-3.91278600	-0.13774400	1.41378200
F	1.25462900	1.91917300	3.74606100
F	1.91504400	2.13336000	1.69147300
F	0.45419400	3.51413700	2.50703800

$[MnO_4/Sc(OTf)_3/3TFA]^-$

Mn	-0.53865600	-3.36246000	0.11976500
O	-0.51405200	-4.25451400	-1.16768000
O	0.86847700	-3.44455700	0.85471000
O	-0.80514500	-1.81829800	-0.31750000
O	-1.70706300	-3.83506100	1.08778300
Sc	0.29256000	-0.04475700	-0.65401300
O	1.24053900	-0.47803400	1.13013300
O	1.62094000	1.45500300	-1.13491200
O	-0.97921800	0.31878800	-2.22676500
S	3.14481700	1.64452100	-1.15738000
S	-2.49437900	0.22818200	-2.46335800
S	0.97718700	-0.36291900	2.63837300
O	3.86218700	0.45571700	-0.66122200
O	3.59974200	2.27329300	-2.40117800
O	-3.23316000	-0.13818400	-1.24660500
O	-2.81155200	-0.45792700	-3.71898700
O	0.09853000	-1.41954000	3.14973600
O	0.69800000	1.02477000	3.04445100
C	2.70031400	-0.77363500	3.27231800
C	3.36342300	2.94890300	0.18137200
C	-2.89368700	2.04679500	-2.74034300
F	2.68294000	-0.78306900	4.60434000
F	3.06178300	-1.97869300	2.83073800
F	3.57937300	0.12863500	2.85156300
F	-2.58202600	2.74883400	-1.64946600
F	-4.19722000	2.17485900	-2.98176000
F	-2.20681300	2.52104300	-3.77546500
F	2.74353500	4.07208200	-0.17430000
F	2.86675400	2.51435800	1.33279600
F	4.66510800	3.19726900	0.32890100
C	3.86050500	-1.97292100	-2.52360300

C	2.76525600	-1.96717000	-1.42428000
O	3.05328000	-2.73021800	-0.42978400
H	2.26953400	-2.89114300	0.17638700
O	1.72343100	-1.35212600	-1.60409400
F	5.08396500	-1.96051400	-2.00080300
F	3.71606600	-0.93933900	-3.34336400
F	3.71622100	-3.10563200	-3.23728800
C	-5.32217400	-0.66234100	0.85335900
C	-3.99193900	-1.42500000	1.09306900
O	-4.04684700	-2.64829800	0.66842300
H	-3.19807400	-3.13785100	0.86193400
O	-3.06627700	-0.91403000	1.69198300
F	-5.89905000	-0.98443700	-0.30047700
F	-5.11870900	0.65467400	0.89208900
F	-6.17106200	-0.98309300	1.85038200
C	-1.05976200	3.34781500	1.57173400
C	-1.48812600	1.87063100	1.36821100
O	-2.45204700	1.51401800	2.12688300
H	-2.75415300	0.55052300	1.95770600
O	-0.95264400	1.19328100	0.50114800
F	0.10048300	3.58564200	0.97174500
F	-0.95786400	3.65099000	2.86484300
F	-1.99643000	4.14107900	1.02205600

$[MnO_3/Sc(OTf)_3/3TFA]^-$

Mn	1.52297800	-0.43665500	2.26791700
O	1.16108700	-1.93371800	3.04377800
O	2.99517500	-0.07410000	2.03775100
O	0.21774100	0.69532700	1.83177500
O	1.45048700	0.30229700	4.11005400
C	2.14275200	1.53181500	4.43149100
H	1.84620900	1.83809100	5.43928000
H	1.81801600	2.27562100	3.69952000
H	3.22587400	1.37837100	4.36191400
H	1.60683000	-0.39778100	4.76317200
Sc	-0.73558000	0.21140800	-0.02662300
O	-1.64650000	0.05825300	-1.83876600
O	0.52843100	1.63442500	-0.88674300
O	-1.74620600	-1.47350400	0.61972600
S	1.30189100	2.81637000	-0.31977800
S	-1.77563300	-2.76074500	1.43236700
S	-2.79791900	-0.44729800	-2.71453500
O	0.53798700	3.65888200	0.60315700
O	2.66775800	2.41720800	0.11192000
O	-2.50005600	-2.61386800	2.69805500
O	-0.44733800	-3.42533500	1.47207400
O	-2.97724400	-1.90044200	-2.62324500
O	-2.77320800	0.18415000	-4.03960200
C	-4.28205100	0.30062800	-1.82365800
C	1.56368400	3.82574900	-1.88414900
C	-2.82324500	-3.88044400	0.34049100
F	-5.39380900	-0.02684500	-2.48391400
F	-4.35772900	-0.17547200	-0.58288500
F	-4.17594000	1.62654000	-1.78062200
F	-3.99070600	-3.29862500	0.09480600
F	-3.02998600	-5.02410300	0.99503500

F	-2.19227800	-4.13399400	-0.79527800
F	2.23356800	3.10325200	-2.77732500
F	0.38863700	4.18185100	-2.39087300
F	2.26489800	4.91601400	-1.58238900
C	5.75246000	-1.09541800	-1.05884800
C	5.08024500	0.19782100	-0.51702900
O	3.79629400	0.21840800	-0.78761900
H	3.37045200	1.05323400	-0.42985300
O	5.71794700	1.02160600	0.08731400
F	5.60067700	-2.09100300	-0.16886900
F	7.06197900	-0.89921900	-1.24097300
F	5.22215500	-1.49066800	-2.22255400
C	1.47835700	-2.20892200	-1.60359400
C	1.82459900	-2.01812700	-0.09984800
O	2.64657200	-2.70972000	0.43438000
H	0.75554800	-2.61546800	2.44943000
O	1.11698000	-1.05998000	0.46331900
F	1.17367000	-1.03612100	-2.18616000
F	0.41024600	-3.01509900	-1.71900200
F	2.49558100	-2.75532500	-2.25907800
C	-3.44703900	3.23954100	1.64307300
C	-2.23012200	2.27490200	1.73850300
O	-1.55051500	2.27437100	2.76294900
H	-0.28371200	1.29873300	2.45819000
O	-2.08309300	1.56155100	0.69530500
F	-3.32964500	4.03739200	0.56955300
F	-3.55884500	4.01382000	2.72592000
F	-4.58648700	2.53661000	1.51431900

INT1[Sc(OTf)$_3$/3TFA]

Mn	-0.53347500	-3.06893800	1.27504500
O	-0.55332800	-4.37913400	0.41742100
O	0.88947200	-2.90221000	1.96126700
O	-0.78611700	-1.80152300	0.28278200
O	-1.68878300	-3.11824600	2.36600300
Sc	0.27543100	-0.16861400	-0.53848100
O	1.24684700	-0.04739700	1.28249500
O	1.59779700	1.12173000	-1.44557000
O	-0.99708600	-0.24644000	-2.14927200
S	3.11862600	1.26366800	-1.60251500
S	-2.49924100	-0.45670200	-2.38724300
S	1.03160200	0.53758600	2.68453400
O	3.86037200	0.28278700	-0.78966800
O	3.50906500	1.45482300	-3.00298700
O	-3.24409000	-0.64385700	-1.13425100
O	-2.75751300	-1.36650300	-3.50604100
O	0.17893000	-0.30216700	3.53179600
O	0.75266300	1.98313700	2.64238700
C	2.77626900	0.34638300	3.36238300
C	3.40572500	2.92357800	-0.76375800
C	-2.98951600	1.25517500	-2.99915900
F	2.79348000	0.74276700	4.63409600
F	3.14125600	-0.93427000	3.29801600
F	3.63263200	1.08149800	2.66230300
F	-2.75874900	2.16582700	-2.05143300
F	-4.28889900	1.25534600	-3.29166900

F	-2.29430200	1.57381700	-4.08720100
F	2.76100000	3.88313600	-1.42425200
F	2.97701300	2.88541200	0.49183600
F	4.71233800	3.18953600	-0.77467800
C	3.78073900	-2.64720100	-1.80651700
C	2.72503200	-2.26731800	-0.73505400
O	3.02447600	-2.70770600	0.43609100
H	2.26278600	-2.64278300	1.08667700
O	1.70244100	-1.68871500	-1.06885000
F	5.02184700	-2.49752600	-1.34997100
F	3.62109400	-1.92247000	-2.90634300
F	3.59774700	-3.94390300	-2.12016600
C	-5.30412100	-0.27664900	1.01074100
C	-3.98526800	-0.92536900	1.50793400
O	-4.04029100	-2.21989900	1.51224000
H	-3.19537100	-2.60978800	1.87590700
O	-3.06442200	-0.24787400	1.92068900
F	-5.89821300	-0.98247900	0.05404200
F	-5.07713600	0.96148700	0.57002700
F	-6.14786500	-0.19745900	2.05947200
C	-0.97502800	3.74193900	0.61121100
C	-1.45429700	2.28494300	0.84485600
O	-2.42568900	2.19590100	1.67058100
H	-2.75301400	1.23184000	1.77663400
O	-0.95453300	1.36419700	0.21188500
F	0.19945900	3.75679200	-0.00641700
F	-0.88113100	4.41455600	1.75676700
F	-1.87736700	4.36175400	-0.17104900
C	-0.21532100	-3.58407400	-2.78328700
H	-0.75092100	-3.26806200	-1.88126800
H	0.60335900	-4.25664600	-2.50092800
H	-0.91179400	-4.10387400	-3.45083100
H	0.18718400	-2.69924100	-3.28914000

INT2[Sc(OTf)$_3$/3TFA]

Mn	-0.41437100	-3.25696100	0.78999900
O	-0.41765900	-4.42108300	-0.49333300
O	1.03972100	-3.19577600	1.42739600
O	-0.71839500	-1.87834200	-0.07917400
O	-1.62731500	-3.54169600	1.77530100
Sc	0.27759800	-0.13950000	-0.55818100
O	1.27564300	-0.22663600	1.25158600
O	1.57814300	1.31342500	-1.28565200
O	-1.02007300	0.07735800	-2.15908400
S	3.09038300	1.54506500	-1.34647500
S	-2.54469600	0.07924600	-2.31286200
S	1.01954100	0.08808200	2.73033100
O	3.85465600	0.46537100	-0.69292000
O	3.52510500	2.00484000	-2.67051000
O	-3.24402600	0.05342500	-1.01940700
O	-2.99449600	-0.83419600	-3.37028100
O	0.15856100	-0.90320800	3.38562800
O	0.72410100	1.51265100	2.95588000
C	2.75316900	-0.20617500	3.39985100
C	3.27483100	3.03584900	-0.21273400
C	-2.80964900	1.81869000	-2.97796700

F	2.74613100	-0.02625100	4.72052000
F	3.13364300	-1.45518200	3.13166000
F	3.61502100	0.64120500	2.84729600
F	-2.37213200	2.71196700	-2.08975100
F	-4.11029500	2.01375800	-3.18817000
F	-2.15109900	1.98112500	-4.12198800
F	2.62949600	4.08040200	-0.72890200
F	2.78535700	2.76549000	0.99120200
F	4.57000000	3.33668100	-0.10292600
C	3.90562400	-2.21103000	-2.19984800
C	2.81977900	-2.05056700	-1.10406900
O	3.12483900	-2.64097800	-0.00609400
H	2.33604400	-2.73626000	0.62345000
O	1.76589200	-1.49086100	-1.37749700
F	5.13480500	-2.11489500	-1.70060300
F	3.74679800	-1.31377800	-3.16547900
F	3.76145900	-3.43965800	-2.73684900
C	-5.32438800	-0.61614500	1.02347200
C	-3.95119300	-1.26632100	1.34109000
O	-3.93005000	-2.52620200	1.04433000
H	-3.05937400	-2.95137800	1.31796700
O	-3.06212700	-0.64237400	1.88777800
F	-5.83293800	-1.03259900	-0.13392600
F	-5.22621000	0.71251900	1.00912500
F	-6.18445800	-0.95976500	2.00405900
C	-1.13810400	3.59178600	1.11427300
C	-1.51454900	2.08665900	1.14004200
O	-2.49269800	1.83111900	1.92299300
H	-2.77243100	0.84692900	1.91008100
O	-0.92305800	1.29620700	0.42082200
F	-0.00656300	3.78123500	0.44583600
F	-1.00400900	4.07515000	2.35010000
F	-2.11899600	4.27326300	0.49761900
C	-0.61645000	-3.29880600	-3.12366900
H	-0.55224900	-3.98096400	-1.37970000
H	-0.63405400	-4.33054500	-3.47309800
H	-1.53985000	-2.72367100	-3.08976800
H	0.33536500	-2.77284900	-3.07718300

INT3[Sc(OTf)$_3$/3TFA]

Mn	-1.27731200	-1.90606700	2.28454100
O	-1.24821000	-3.43564900	1.43012100
O	0.22199300	-2.26612900	3.20404200
O	-0.97169200	-0.72591700	1.18603200
O	-2.57970600	-1.71326000	3.18180200
Sc	0.37416900	-0.28396600	-0.29920400
O	1.49978600	0.74583900	1.10934300
O	1.77487100	0.00830600	-1.80431100
O	-0.98000900	-1.15581200	-1.63043500
S	3.29039800	-0.15917800	-1.95825100
S	-2.47077900	-1.46243200	-1.50976000
S	1.36169100	2.01097600	1.95662800
O	3.93715300	-0.63604700	-0.72588300
O	3.64586400	-0.79667400	-3.23240900
O	-3.27489900	-0.31049000	-1.08007900
O	-2.72591800	-2.76241400	-0.85218200

O	0.43564000	1.84521100	3.08673200
O	1.22720600	3.22787100	1.13838700
C	3.08228200	2.06743900	2.71412100
C	3.81246300	1.63960700	-2.14155200
C	-2.90319000	-1.73764300	-3.31758600
F	3.16790700	3.12276900	3.52352900
F	3.29463400	0.95726500	3.42185400
F	4.00622100	2.16583400	1.76540500
F	-2.66778800	-0.62585000	-4.00925400
F	-4.19474300	-2.04840300	-3.41072100
F	-2.17463200	-2.73134100	-3.81771400
F	3.24391400	2.17373300	-3.22227500
F	3.45371000	2.33683200	-1.06835900
F	5.13916500	1.69784800	-2.27657400
C	2.85222800	-3.94605800	-0.28490100
C	1.93522500	-3.07255300	0.61550700
O	1.88376100	-3.47862200	1.82228600
H	1.18551800	-2.94877400	2.42184200
O	1.35490200	-2.11137500	0.12668900
F	4.12186500	-3.85370200	0.12947900
F	2.78129600	-3.55858000	-1.55379000
F	2.47667000	-5.23112500	-0.20848600
C	-5.21995100	1.39402700	0.56969600
C	-4.08883200	0.76213900	1.42545800
O	-4.45605500	-0.35331700	1.96719200
H	-3.72261500	-0.79423900	2.50231100
O	-3.03174900	1.34060200	1.59324000
F	-5.96895000	0.48490400	-0.04924000
F	-4.71079400	2.22985400	-0.33693100
F	-6.01929300	2.10624500	1.38990500
C	-0.39844600	3.80985800	-1.51594400
C	-0.98137400	2.71779900	-0.58058300
O	-1.91164300	3.15180800	0.18199900
H	-2.36607600	2.42565400	0.74089800
O	-0.58681800	1.56465200	-0.67995600
F	0.78293600	3.44063500	-1.99653100
F	-0.27435300	4.97990200	-0.89140900
F	-1.24765000	3.97066100	-2.54895300
C	0.70231200	-1.34236300	4.18563600
H	-1.78957400	-3.36516500	0.61261200
H	0.57878000	-0.30630600	3.84950200
H	0.15561400	-1.49720000	5.12526100
H	1.76950100	-1.54839100	4.34009400

TS1[Sc(OTf)$_3$/3TFA]

Mn	-0.47360900	-3.20931500	0.92374800
O	-0.50493100	-4.38732500	-0.27095400
O	0.98255300	-3.13214100	1.55543500
O	-0.76699000	-1.85460300	0.00844000
O	-1.67623900	-3.42833300	1.93885300
Sc	0.25831400	-0.16158900	-0.54404300
O	1.27495600	-0.19462300	1.25821400
O	1.58560200	1.23971900	-1.33057500
O	-0.99605600	-0.00013500	-2.18618400
S	3.10184800	1.42298900	-1.43137800
S	-2.51652900	-0.00186800	-2.37776700

S	1.05382500	0.20601800	2.72074600
O	3.84869500	0.35156700	-0.74452300
O	3.52371500	1.80985100	-2.78281500
O	-3.24454700	-0.09704400	-1.10374300
O	-2.93206200	-0.86518400	-3.48942300
O	0.19330400	-0.73231800	3.45007400
O	0.78113900	1.64588200	2.86764500
C	2.79424600	-0.07642600	3.37733700
C	3.35206700	2.95766600	-0.37168500
C	-2.78800300	1.76350900	-2.96947400
F	2.80754800	0.15987700	4.68917700
F	3.15767700	-1.33994400	3.15788200
F	3.65680400	0.73713600	2.77780700
F	-2.39155300	2.62333500	-2.03037700
F	-4.08515700	1.94901300	-3.20917700
F	-2.09933700	1.98769200	-4.08503000
F	2.71697500	3.99367700	-0.91770200
F	2.89012600	2.75417200	0.85578300
F	4.65647700	3.23180100	-0.31015200
C	3.80730800	-2.37824200	-2.16681300
C	2.74415600	-2.14857300	-1.06103500
O	3.05230100	-2.70666400	0.05325900
H	2.27571500	-2.75269800	0.70311600
O	1.70214300	-1.56907600	-1.33806100
F	5.04671500	-2.28436600	-1.69249900
F	3.64818800	-1.51966300	-3.16696100
F	3.63203700	-3.62552400	-2.64814900
C	-5.32097600	-0.48392100	1.01417100
C	-3.96635900	-1.14613300	1.38187200
O	-3.96508800	-2.42000100	1.15274300
H	-3.10428100	-2.84383300	1.45804300
O	-3.07335200	-0.51098900	1.90881400
F	-5.85450900	-0.98513800	-0.09684900
F	-5.18018000	0.83454900	0.87992700
F	-6.18129700	-0.70932800	2.02857500
C	-1.02625100	3.63363200	1.03616200
C	-1.46826300	2.14748500	1.09904400
O	-2.44243300	1.94728300	1.90307300
H	-2.75741900	0.97372500	1.90853400
O	-0.93273000	1.31782700	0.37874400
F	0.12468000	3.75377400	0.38630200
F	-0.90003300	4.15471800	2.25638100
F	-1.96641000	4.33193500	0.37425400
C	-0.94812800	-3.49250500	-2.59463700
H	-0.72736800	-3.90438400	-1.39578400
H	-0.88448900	-4.44505100	-3.12743700
H	-1.94151200	-3.04415500	-2.54802400
H	-0.13870600	-2.78953900	-2.79735800

TS2[Sc(OTf)$_3$/3TFA]

Mn	0.31849800	3.27450600	0.29362400
O	0.19566700	4.15596800	-1.21624500
O	-1.13836000	3.30123600	0.93743400
O	0.70123800	1.76718100	-0.25052700
O	1.49144500	3.86741000	1.18793400
Sc	-0.21447500	-0.03165800	-0.62533200

O	-1.25546900	0.21914600	1.15644600
O	-1.40847300	-1.64959800	-1.16260300
O	1.05894700	-0.30722600	-2.22522200
S	-2.90252900	-1.97610700	-1.22550400
S	2.56552100	-0.13417400	-2.45122000
S	-1.00431000	0.10848500	2.66290500
O	-3.74335800	-0.88018400	-0.70733900
O	-3.27913500	-2.60210200	-2.49827800
O	3.28381700	0.23378800	-1.22217100
O	2.85730400	0.59926700	-3.68701100
O	-0.25982000	1.24939100	3.20914200
O	-0.57665700	-1.24425300	3.05951500
C	-2.77049000	0.31376900	3.27819900
C	-3.02490100	-3.34325200	0.06140300
C	3.05633200	-1.92173100	-2.77625500
F	-2.77173200	0.31195200	4.61116500
F	-3.26226400	1.47488600	2.84342400
F	-3.53851100	-0.67739800	2.83909100
F	2.76808600	-2.67131100	-1.71081500
F	4.36756700	-1.98132000	-3.00653400
F	2.40452600	-2.39851300	-3.83348100
F	-2.28926100	-4.38808300	-0.31513400
F	-2.60044900	-2.90744800	1.24141300
F	-4.29908600	-3.72493000	0.16692800
C	-3.94764600	1.61095300	-2.47814200
C	-2.84272600	1.65092600	-1.39025800
O	-3.17907000	2.35432900	-0.36887200
H	-2.39562400	2.58859600	0.22700000
O	-1.75913600	1.12558700	-1.60327700
F	-5.16104300	1.47648200	-1.94751400
F	-3.73158300	0.63138400	-3.34641500
F	-3.90692900	2.78431000	-3.14184400
C	5.30807200	0.97823400	0.84782900
C	3.91666100	1.62019500	1.09342000
O	3.85537500	2.83797400	0.66071000
H	2.96465000	3.25827800	0.86603900
O	3.04925900	1.03100700	1.70970200
F	5.84618700	1.33922400	-0.31359100
F	5.22904700	-0.35158400	0.90251400
F	6.13295700	1.38653600	1.83456000
C	1.38871900	-3.37867300	1.57051700
C	1.68710000	-1.86932900	1.37083300
O	2.62071500	-1.43508700	2.12843800
H	2.84645700	-0.45000300	1.95996800
O	1.09145600	-1.24033500	0.50823700
F	0.23666600	-3.70980700	1.00022100
F	1.34880600	-3.70185200	2.86278100
F	2.37348200	-4.08667700	0.98755000
C	-2.54050800	5.56173300	-0.15837300
H	-0.24890200	5.00995400	-1.07134000
H	-2.79750200	5.15413800	-1.13401300
H	-3.03644200	5.18983700	0.73415400
H	-1.87784600	6.42249300	-0.08134200

TS3[Sc(OTf)$_3$/3TFA]

Mn	0.42225900	3.36032500	-0.66925400

O	-0.28682200	4.16806100	-1.95261400
O	-1.40679700	3.68130500	-0.04395400
O	0.59843400	1.71696100	-0.85599600
O	1.53970900	4.14414200	0.16140000
Sc	-0.24500500	-0.10776800	-0.74265100
O	-1.29988900	0.52664900	0.95094600
O	-1.41197500	-1.85053000	-0.88362000
O	1.10254300	-0.79939500	-2.15567400
S	-2.88561700	-2.22306300	-0.73206600
S	2.61980500	-0.66652800	-2.32530500
S	-1.02013400	0.82876400	2.42306400
O	-3.74077100	-1.05249300	-0.45255800
O	-3.32970800	-3.17570600	-1.75687400
O	3.27722600	-0.08617400	-1.14382300
O	2.98754500	-0.16465400	-3.65361900
O	-0.35481800	2.12579900	2.61887500
O	-0.49722200	-0.32923300	3.16229900
C	-2.78506200	1.08131100	3.02372500
C	-2.85318500	-3.20044900	0.87784600
C	3.11103700	-2.48259900	-2.30129600
F	-2.76375000	1.42630400	4.31090500
F	-3.35921900	2.06400800	2.32234200
F	-3.49690800	-0.02969800	2.87979100
F	2.75783100	-3.03230000	-1.13634500
F	4.43195600	-2.58292200	-2.44348300
F	2.51329700	-3.14078200	-3.29066900
F	-2.21917700	-4.35732500	0.69545300
F	-2.23579300	-2.50721600	1.82913600
F	-4.10673400	-3.44911100	1.26089100
C	-4.12841100	0.89053700	-2.75829200
C	-2.99124200	1.22097700	-1.75663600
O	-3.34054800	2.10129900	-0.88270400
H	-2.56524700	2.49093800	-0.38195900
O	-1.88262600	0.73321000	-1.91014100
F	-5.31772200	0.84198800	-2.16295100
F	-3.89597200	-0.25831600	-3.38098200
F	-4.15877500	1.87427800	-3.67921100
C	5.27798900	1.15307800	0.79259500
C	3.88194700	1.82846600	0.87038200
O	3.85524000	2.95069700	0.22930700
H	2.95487900	3.40447900	0.28230400
O	2.98219500	1.35347100	1.53748100
F	5.83076000	1.25950300	-0.41328900
F	5.19963800	-0.13496100	1.12700100
F	6.08959800	1.76471900	1.67963200
C	1.40838200	-3.07013100	1.90678600
C	1.66554100	-1.57956200	1.55647200
O	2.59114400	-1.05306600	2.26566600
H	2.78559800	-0.08397600	2.00115400
O	1.02583700	-1.03986400	0.66923400
F	0.55078800	-3.60825400	1.04625500
F	0.90891700	-3.17692300	3.14236200
F	2.55786700	-3.75755300	1.85436000
C	-1.65441400	4.57843700	1.06589400
H	-1.29276100	4.16629300	-1.07691600
H	-2.73905000	4.71658100	1.13971500

H	-1.26111800	4.11124400	1.96995700
H	-1.16307400	5.53948900	0.87701800

[MnO_4/Sc(OTf)$_2$]

Sc	0.03607800	0.48584700	-0.21575900
O	0.25312800	2.51673400	-0.83637900
O	1.72896000	1.31850100	0.76725500
Mn	1.59175600	2.79176500	0.06575600
O	2.82566900	3.12059000	-0.82555000
O	1.36079200	3.91077800	1.12221400
O	-1.85303400	0.43021100	-1.33581300
O	-1.69916800	0.78033800	1.00932800
O	0.46381300	-1.30360600	1.00560800
O	0.87353000	-1.14499500	-1.32703200
S	0.99373300	-2.12838800	-0.15764700
S	-2.73198100	0.66892300	-0.11419200
C	2.85231200	-2.28893300	0.14179400
C	-3.58286900	-0.98968900	0.19805900
O	0.47425800	-3.46975700	-0.35039700
O	-3.76564100	1.68407300	-0.19053200
F	-2.66231600	-1.93382100	0.33434500
F	-4.30319500	-0.89464500	1.30431400
F	-4.36457700	-1.26171400	-0.83534500
F	3.38194600	-1.08339900	0.27601500
F	3.03771700	-2.99437500	1.24682900
F	3.39323400	-2.91167700	-0.89418900

[MnO_3/Sc(OTf)$_2$]

Sc	-0.08349500	-0.33773900	-0.18400000
O	-1.89989300	-0.73450500	-1.32650000
O	1.70913400	-0.89346400	-1.30297700
S	2.35751000	-1.69844000	-0.17943100
S	-2.66350000	-1.41836900	-0.19407400
O	1.33496300	-1.58764100	0.94344200
O	2.88547900	-3.01223100	-0.50274600
O	-1.66582100	-1.37431900	0.95437900
O	-3.32140000	-2.68009000	-0.48636600
C	-4.01843200	-0.18974800	0.28127700
C	3.81841700	-0.64144000	0.38679400
F	-4.67235500	-0.67103100	1.32836600
F	-3.47542900	0.98050800	0.58607300
F	-4.84377600	-0.05092800	-0.74623300
F	4.67872800	-0.53226200	-0.61445400
F	3.38496200	0.56075300	0.74297700
F	4.39512900	-1.23645300	1.42041200
Mn	0.46230100	3.15038200	-0.07718300
O	1.28918500	3.48633900	-1.36192600
O	0.00272700	1.50278800	0.19090000
O	-0.19856400	4.25984200	0.80516500

INT1[Sc(OTf)$_2$]

Sc	-0.07234900	-0.13422300	-0.39306000
O	1.12962800	-1.41020700	0.90712400
O	-1.67396800	-0.29664300	1.07842400
S	-2.43142200	-1.39917900	0.34736000
S	2.14954500	-1.77782100	-0.16306200

O	-1.53536400	-1.65354400	-0.86592200
O	-2.89693000	-2.54472700	1.10514200
O	1.61692700	-1.01485200	-1.37859000
O	2.50372500	-3.17407800	-0.33420500
C	3.72383500	-0.84819200	0.31622600
C	-3.94889800	-0.52715900	-0.36710000
F	4.61783400	-1.00739100	-0.64751500
F	3.44184900	0.43746100	0.46738000
F	4.18109800	-1.35052600	1.45230100
F	-4.72664400	-0.14152100	0.63205100
F	-3.55088600	0.52943800	-1.06614200
F	-4.59744800	-1.37154300	-1.15302800
Mn	0.54822900	2.58365400	-0.48206900
O	0.67264600	1.51508500	0.74356600
O	-0.47868900	3.70799600	-0.15252500
C	-1.06272200	2.44117500	3.16507200
H	-1.56260700	2.83321000	4.05951600
H	-0.00957200	2.23158700	3.38948700
H	-1.55094200	1.51509900	2.84109300
H	-1.12098400	3.18367600	2.35851400
O	-0.02177500	1.56527400	-1.63888900
O	1.93408200	3.18538700	-0.85687500

INT2[Sc(OTf)$_2$]

Sc	0.10521200	-0.39104700	-0.42972300
O	1.55145400	-1.56780500	0.75513000
O	-1.38052000	-1.08760900	1.04635600
S	-2.32535500	-1.71245600	0.02958800
S	2.69764500	-1.42934100	-0.23571000
O	-1.60718800	-1.47036000	-1.29234700
O	-2.84454600	-3.04233900	0.29602500
O	2.06391500	-0.61789300	-1.36185400
O	3.44817900	-2.62145200	-0.59198200
C	3.91319100	-0.23633200	0.57961200
C	-3.79680600	-0.53262500	-0.01297400
F	4.88589900	0.03089800	-0.28058500
F	3.28237200	0.87982700	0.91124500
F	4.41208100	-0.81453900	1.66322400
F	-4.37806800	-0.52987000	1.17874100
F	-3.36000000	0.68872200	-0.30084900
F	-4.65357600	-0.93599500	-0.93691600
Mn	0.02656700	2.39977800	-0.52931200
O	0.37197000	1.29815600	0.68676400
O	-1.41290200	3.11048200	0.07452200
C	-2.08634100	1.92295700	2.57367900
H	-3.12065200	2.25295100	2.47378200
H	-1.37754600	2.55087000	3.11127900
H	-1.82863500	0.88527600	2.37282400
H	-1.74609400	2.67338600	0.91485900
O	-0.22204400	1.26669900	-1.69488400
O	1.20218400	3.39817400	-0.70191300

INT3[Sc(OTf)$_2$]

Sc	-0.02337300	-0.35707900	-0.49432000
O	1.42351100	-1.46883200	0.81662500
O	-1.51465800	-0.84026100	1.09993600

S	-2.47334300	-1.56402900	0.17318200
S	2.48713400	-1.60569100	-0.25576000
O	-1.77054400	-1.47642500	-1.17781500
O	-2.99745100	-2.85678300	0.58098700
O	1.83561800	-0.95375900	-1.47199600
O	3.12499000	-2.89917200	-0.43919600
C	3.84310800	-0.39400200	0.25108000
C	-3.95035300	-0.40034200	0.01420600
F	4.80298800	-0.41139200	-0.66201500
F	3.33265200	0.82722700	0.34541900
F	4.32962100	-0.76917800	1.42704400
F	-4.59769000	-0.37434600	1.17162100
F	-3.52006200	0.81992300	-0.28469200
F	-4.75100200	-0.84326400	-0.94354000
Mn	0.02074800	2.55057000	-0.37198400
O	0.40362400	1.22618000	0.81923900
O	-1.40273400	3.28306700	0.33243200
C	0.57816000	1.38727000	2.22318800
H	0.84293800	0.40558200	2.63301700
H	-0.35023300	1.74326100	2.68744200
H	1.38851100	2.10124600	2.41209600
H	-1.87785300	2.77360000	1.00784300
O	-0.27864600	1.33325800	-1.51941200
O	1.24555000	3.48122300	-0.56007500

TS1[Sc(OTf)$_2$]

Sc	-0.02354400	-0.09298000	-0.37133400
O	1.19761300	-1.40726900	0.91910000
O	-1.67367500	-0.25027000	1.07054600
S	-2.34142300	-1.45438300	0.41416300
S	2.20946500	-1.74580900	-0.16205800
O	-1.42584500	-1.74185000	-0.76823700
O	-2.74461000	-2.56390300	1.25947000
O	1.67617100	-0.97390400	-1.36947200
O	2.57995500	-3.13645900	-0.35707600
C	3.78012600	-0.81643500	0.32467900
C	-3.90210600	-0.74067500	-0.36849900
F	4.67626600	-0.96129000	-0.64136800
F	3.49914600	0.46716400	0.49263800
F	4.24343900	-1.33067400	1.45503800
F	-4.72819800	-0.35285500	0.59235800
F	-3.56541000	0.29967300	-1.12174700
F	-4.47698000	-1.67157300	-1.11476300
Mn	0.42189900	2.64516900	-0.49395600
O	0.69208900	1.50568000	0.69994100
O	-0.73661100	3.58782800	0.23195100
C	-1.31241100	2.77296100	2.58119800
H	-2.00423600	3.55875700	2.89910800
H	-0.35541600	2.75207300	3.10745500
H	-1.75960500	1.79172300	2.40759500
H	-1.02689500	3.17769800	1.42929000
O	-0.16877100	1.59898200	-1.62035300
O	1.72573400	3.43080400	-0.80510600

TS2[Sc(OTf)$_2$]

Sc	0.04371100	-0.35181700	-0.41310100

O	1.46248400	-1.56365600	0.78108600
O	-1.45257300	-1.01232900	1.06624400
S	-2.39597600	-1.65094700	0.05609400
S	2.58784200	-1.51688300	-0.24003100
O	-1.66632100	-1.44155600	-1.26521000
O	-2.92492700	-2.97202700	0.34693500
O	1.96878900	-0.71316500	-1.37954200
O	3.27170600	-2.75569200	-0.57074400
C	3.87722800	-0.35452500	0.50129700
C	-3.86215400	-0.46542700	-0.01952000
F	4.83844900	-0.16235900	-0.39133300
F	3.30515000	0.80088700	0.80647200
F	4.37804200	-0.91463600	1.59366900
F	-4.46481100	-0.45653400	1.16154700
F	-3.42067700	0.75314800	-0.30731800
F	-4.70341200	-0.87484300	-0.95606400
Mn	0.12230100	2.43516200	-0.54121200
O	0.38214000	1.33394800	0.70226200
O	-1.23648000	3.24448100	0.13779900
C	-1.38528500	1.89509700	2.73424000
H	-1.61899000	0.85763600	2.51000900
H	-2.19301100	2.62540000	2.80758100
H	-0.40092800	2.15254700	3.11742000
H	-1.49638600	2.83549500	1.00492300
O	-0.24446100	1.29696800	-1.67559300
O	1.37596900	3.32821600	-0.73703400

TS3[Sc(OTf)$_2$]

Sc	-0.01909500	-0.42542000	0.18323200
O	1.84377200	-0.92580200	1.23845800
O	-1.91874100	-0.40754900	1.27597500
S	-2.61411100	-1.45031100	0.40897800
S	2.51859800	-1.63257600	0.06617700
O	-1.52185800	-1.83986600	-0.57703600
O	-3.35022800	-2.51273700	1.07341500
O	1.45816200	-1.57574800	-1.01805000
O	3.18112900	-2.89957200	0.32557200
C	3.85202600	-0.41524200	-0.48835800
C	-3.86188800	-0.45654700	-0.60099500
F	4.36271200	-0.82754500	-1.63801800
F	3.31320600	0.79057600	-0.63991800
F	4.79848100	-0.36624400	0.43889200
F	-4.76444200	0.05226700	0.22658000
F	-3.23291500	0.51754000	-1.24007300
F	-4.44983800	-1.26559100	-1.47096000
Mn	-0.04757200	2.55701100	-0.31577000
O	0.18166200	1.42685700	1.42210500
O	-1.36276700	2.93750800	0.63891300
C	1.18196400	1.74417500	2.41638100
H	1.03266600	1.08150300	3.27546700
H	1.06237800	2.79036200	2.71703100
H	2.17185200	1.58006100	1.98183700
H	-0.78832700	2.08132000	1.43905500
O	-0.19340500	1.03457600	-1.09279200
O	0.72758500	3.69460100	-1.03908400

INT1′[Sc(OTf)$_2$]

Sc	-0.08064000	-0.11936600	-0.64530000
O	0.89572200	-1.61114100	0.58976500
O	-2.11635100	-0.09845600	-1.36393300
S	-2.78347000	-0.09058600	0.01544400
S	1.94502100	-2.01123900	-0.44523900
O	-1.58581500	-0.05622000	0.95344500
O	-3.87128700	0.84210300	0.23879400
O	1.56676100	-1.13759700	-1.63914200
O	2.17529000	-3.42567900	-0.67453000
C	3.56018300	-1.26168900	0.18652700
C	-3.47752300	-1.83875200	0.19262800
F	4.50716300	-1.48266000	-0.71216300
F	3.39079500	0.03994300	0.35982300
F	3.87639200	-1.83863100	1.33516000
F	-4.46706300	-1.99511600	-0.67290800
F	-2.51069600	-2.71268600	-0.06132600
F	-3.92082000	-1.99973700	1.42879700
Mn	0.31702900	3.20342000	-0.21345400
O	0.77902700	1.57674900	-0.38143000
O	0.35040200	3.56702500	1.30615300
C	1.15849200	0.75252600	3.05123400
H	1.31827900	1.27801200	4.00020200
H	1.56423400	-0.26458300	3.11290500
H	0.08455100	0.70199800	2.83549000
H	1.66142100	1.29619200	2.24228900
O	-1.12747900	3.38751900	-0.78664000
O	1.33692400	4.08397900	-1.00564700

INT2′[Sc(OTf)$_2$]

Sc	-0.03363700	-0.09797900	-0.76440200
O	0.94903400	-1.40743900	0.68146600
O	-2.08825100	-0.29208600	-1.47145900
S	-2.75356400	-0.15041200	-0.10295500
S	1.94625000	-2.00660300	-0.30287000
O	-1.56161600	0.01331100	0.82624600
O	-3.86605600	0.77357500	0.02157500
O	1.55781700	-1.32773500	-1.61268400
O	2.12778300	-3.44721100	-0.30838400
C	3.60616200	-1.23097400	0.15371000
C	-3.41377700	-1.87859500	0.26680800
F	4.49496000	-1.55032500	-0.77426800
F	3.46572300	0.08566000	0.21572900
F	3.98663200	-1.70301000	1.33144600
F	-4.37399600	-2.16632800	-0.59952000
F	-2.42304300	-2.75414100	0.15130800
F	-3.89312900	-1.89853900	1.50122700
Mn	0.25641700	3.20497800	-0.23952200
O	0.76714700	1.55920900	-0.33595600
O	0.24153000	3.38317700	1.48679600
C	0.88765100	0.97407300	2.94114900
H	0.97523100	1.57550200	3.84472700
H	1.78724300	0.67969500	2.40507600
H	-0.05597600	0.48279000	2.71153300
H	0.47553900	2.53213400	1.95233100
O	-1.19740500	3.34488700	-0.80095300

O	1.34957000	4.13385500	-0.85955800

INT3′[Sc(OTf)$_2$]

Sc	0.43481800	-0.02083200	-0.40027600
O	-0.26412300	1.47726600	1.05630800
O	2.27835700	-0.78038100	-1.29913300
S	3.02847100	-0.95848500	0.01769800
S	-0.79429700	2.45964800	0.02111100
O	2.00117700	-0.51486800	1.05006300
O	3.73612100	-2.20745500	0.23590300
O	-0.46093500	1.76970200	-1.29940200
O	-0.44169900	3.86202100	0.16136500
C	-2.67651700	2.35029700	0.16312500
C	4.31343100	0.42343400	0.01605100
F	-3.21749500	3.09096600	-0.79391000
F	-3.06318200	1.08972400	0.03064600
F	-3.03666300	2.81003900	1.35265100
F	5.17583500	0.21054500	-0.96675900
F	3.69528800	1.58392500	-0.16953500
F	4.94261400	0.42896600	1.18114300
Mn	-1.94580600	-2.45414800	0.30837900
O	-0.73164000	-1.48020300	-0.44586100
O	-2.33154500	-1.93210700	1.94014500
C	-3.49777800	-1.70043800	-1.82175600
H	-4.48965700	-1.28413700	-2.04803100
H	-3.38818800	-2.67020600	-2.33144600
H	-2.71989000	-1.01113300	-2.18596600
H	-3.17942700	-1.46028900	1.97960500
O	-1.83906100	-3.99376600	0.11886600
O	-3.41640700	-1.84631900	-0.41718400

TS1′[Sc(OTf)$_2$]

Sc	-0.04045300	-0.12433900	-0.76990600
O	0.95858700	-1.39373000	0.70355000
O	-2.09787800	-0.30919000	-1.47343100
S	-2.75889100	-0.14045900	-0.10632200
S	1.94890500	-2.01493900	-0.27384400
O	-1.56454900	0.02426300	0.81935300
O	-3.86240100	0.79569600	0.00726900
O	1.55299200	-1.36901100	-1.59759600
O	2.13156800	-3.45541900	-0.24602000
C	3.61036800	-1.23040600	0.16001800
C	-3.43165300	-1.85785700	0.28507300
F	4.50124000	-1.58484800	-0.75324500
F	3.47646700	0.08807900	0.17781700
F	3.98467400	-1.66423300	1.35465000
F	-4.39095400	-2.15180300	-0.58031600
F	-2.44428800	-2.73933800	0.18298500
F	-3.91460600	-1.86036900	1.51823600
Mn	0.26712500	3.17757900	-0.22824400
O	0.77526800	1.53217100	-0.39130700
O	0.24268000	3.30193800	1.44812800
C	0.87181200	1.22839400	2.74362300
H	1.04610600	1.69718600	3.71555400
H	1.75652900	0.82412100	2.24990400
H	-0.02595800	0.61136500	2.67076000

H	0.55640400	2.26941000	2.04594600
O	-1.17664400	3.33469200	-0.81214000
O	1.36314100	4.11706200	-0.82765900

TS2′[Sc(OTf)$_2$]

Sc	0.57721400	0.21213600	-0.78144700
O	-0.37274900	1.27378200	0.88257000
O	2.59190700	-0.33791500	-1.47251300
S	3.08879600	-0.81509200	-0.11032800
S	-1.03974500	2.33884900	0.02724900
O	1.88117000	-0.59695700	0.78772200
O	3.78035600	-2.09050700	-0.04630700
O	-0.54659400	1.99894600	-1.37610000
O	-0.95143300	3.72221400	0.46388800
C	-2.87771400	1.88812200	0.00033300
C	4.31222300	0.51530300	0.42943900
F	-3.54078900	2.86100500	-0.60981600
F	-3.04726300	0.75117900	-0.65663600
F	-3.30715900	1.76073800	1.24738200
F	5.33201900	0.53534600	-0.41677400
F	3.69774500	1.69337900	0.42356400
F	4.74043600	0.23765000	1.65145600
Mn	-1.59399600	-2.33494600	-0.09106900
O	-0.59627700	-1.24123400	-0.98206200
O	-1.95488100	-1.39503400	1.34378700
C	-5.04801200	-1.70514800	0.86651000
H	-5.29435400	-2.73223500	0.60925100
H	-5.08365100	-0.93201000	0.10341600
H	-4.94033900	-1.42460600	1.91496800
H	-2.89161800	-1.52762500	1.58987300
O	-0.84110500	-3.63570300	0.32735600
O	-2.99544000	-2.52111300	-0.76976500

TS3′[Sc(OTf)$_2$]

Sc	0.50076600	0.01213900	-0.47722700
O	-0.12632800	1.51972200	0.98166900
O	2.32067800	-0.80811900	-1.36109300
S	3.00509500	-1.13294100	-0.03596900
S	-0.59287300	2.54841300	-0.04042800
O	1.97710800	-0.69513500	0.99592400
O	3.62105300	-2.44017800	0.10835200
O	-0.33449300	1.84799900	-1.37007500
O	-0.12773200	3.91716300	0.10934200
C	-2.47367200	2.58668300	0.13277100
C	4.37301600	0.15731700	0.10072200
F	-2.96351800	3.42491900	-0.77059600
F	-2.96481600	1.37312000	-0.06500800
F	-2.77704200	3.00576200	1.35257600
F	5.23253500	-0.01191500	-0.89343000
F	3.82513500	1.36509000	0.02381900
F	4.98905300	0.01489500	1.26420700
Mn	-1.99102100	-2.25899100	0.31168500
O	-0.71115300	-1.40829200	-0.49451000
O	-2.78054500	-1.42158700	1.53353800
C	-4.54192000	-2.62085100	-1.06299800
H	-5.41280700	-2.04881600	-1.40926300

H	-4.85023100	-3.33725500	-0.28960000
H	-4.08951400	-3.15493000	-1.90659800
H	-3.64750500	-1.32475200	0.59543800
O	-1.93778000	-3.80987400	0.44108100
O	-3.59490100	-1.68266000	-0.53986400

[MnO_4/Sc(OTf)$_2$/3TFA]

Mn	0.79563300	-1.40467600	2.61381000
O	0.78123200	-2.95455300	2.78986300
O	2.29346000	-0.88472100	2.55934300
O	0.05363200	-1.03091600	1.18808600
O	-0.00295400	-0.70857700	3.78205900
Sc	0.53207900	-0.55196700	-0.68990200
O	1.82438600	0.90178200	-0.03562200
O	-0.85620000	-1.87330700	-1.37918900
S	-2.31077800	-2.21924400	-0.98484300
S	1.77967900	2.27807800	0.66113600
O	-2.79838300	-1.35534800	0.09796600
O	-2.51395500	-3.66561700	-0.89997100
O	1.56608400	2.16698500	2.10466700
O	0.97043300	3.24116700	-0.10390900
C	3.57508700	2.78609400	0.42168300
C	-3.21565900	-1.63958800	-2.53242500
F	3.77005000	3.97355400	0.98399000
F	4.37256600	1.88657100	0.99305600
F	3.85536400	2.85894900	-0.87743400
F	-3.01722600	-0.33266700	-2.70612300
F	-4.51566700	-1.87064500	-2.38515200
F	-2.76569000	-2.29538300	-3.59800100
C	4.55346000	-2.37634600	-1.46272400
C	3.49928000	-1.83732800	-0.45483700
O	3.98676900	-1.63958600	0.71201700
H	3.32664800	-1.33330600	1.41060900
O	2.34052900	-1.67384100	-0.82280900
F	5.70806300	-1.72537500	-1.32667100
F	4.11445700	-2.23056800	-2.70917800
F	4.75697600	-3.67660500	-1.22140200
C	-4.38137100	0.46479200	1.91691300
C	-2.88322300	0.35558700	2.30839100
O	-2.68557200	-0.52056800	3.24485600
H	-1.73559300	-0.55213000	3.52126300
O	-2.04234500	1.08516300	1.82070200
F	-4.99917400	-0.71100900	1.93040500
F	-4.50299200	1.01470000	0.70815500
F	-4.98613900	1.27174900	2.80803800
C	-1.16675800	2.99486800	-2.38288900
C	-1.30939000	2.11242300	-1.11539800
O	-2.05272600	2.60866500	-0.21035900
H	-2.13154200	2.00068300	0.61214400
O	-0.78418900	0.99958400	-1.10067900
F	-0.04871800	2.68694100	-3.03753700
F	-1.16143700	4.28864000	-2.08535700
F	-2.21338600	2.74093800	-3.18683900

INT1[Sc(OTf)$_2$/3TFA]

Mn	-1.63843500	-2.65569400	1.08674900

O	-1.63393700	-4.02803900	0.33737100
O	-0.35766600	-2.53899500	2.01332900
O	-1.58157400	-1.45735600	-0.04724200
O	-2.96220800	-2.49726700	1.93461800
Sc	-0.06592800	-0.23180600	-0.75368500
O	0.56366500	0.12479000	1.09391900
O	1.48680800	0.68898800	-1.68759200
S	3.03111900	0.63013500	-1.61253100
S	0.14310700	1.01244700	2.29951500
O	3.48347500	-0.24757200	-0.52028900
O	3.62698000	0.48885600	-2.94188500
O	-0.93556900	0.40363100	3.07702000
O	0.02124600	2.41926000	1.89114600
C	1.71411800	0.85471800	3.32777800
C	3.41213300	2.38516600	-1.04608100
F	1.54753200	1.53002600	4.45921100
F	1.92799800	-0.42879400	3.60061800
F	2.74718300	1.34714100	2.65994600
F	3.00444500	3.25288500	-1.96739700
F	2.79679900	2.63362600	0.10324900
F	4.72678600	2.50144100	-0.88083300
C	3.17267400	-3.28992100	-1.05572500
C	2.02316000	-2.63569900	-0.24333700
O	2.07035700	-2.91639100	1.00945800
H	1.23020100	-2.66104100	1.48956100
O	1.14614800	-2.00183900	-0.81836700
F	4.33775800	-3.17582000	-0.42671300
F	3.26045600	-2.74744500	-2.26360300
F	2.88506000	-4.59586700	-1.19215200
C	-4.90564600	0.17042100	-1.41420700
C	-4.48231700	-0.31788000	-0.00244400
O	-4.79643400	-1.56440400	0.18116200
H	-4.37225600	-1.92308700	1.00047800
O	-3.90373000	0.40299600	0.78464000
F	-4.14008000	-0.43331100	-2.33599300
F	-4.72560200	1.48866300	-1.51658500
F	-6.18236300	-0.11449500	-1.66311700
C	-1.02368900	3.84349400	-0.66667100
C	-1.74107500	2.52326900	-0.27818300
O	-2.80456600	2.68858000	0.40159600
H	-3.29348400	1.80898800	0.57043200
O	-1.31641000	1.44539800	-0.70196000
F	0.24743900	3.61195400	-0.96779700
F	-1.09776100	4.74619700	0.30356300
F	-1.64082200	4.33197800	-1.75759100
C	-1.51309400	-3.02548800	-3.05746200
H	-1.51934200	-3.34854300	-2.00853700
H	-1.70071300	-3.89129500	-3.70391500
H	-2.29855200	-2.27564300	-3.21014500
H	-0.53182100	-2.59757800	-3.30160100

TS1[Sc(OTf)$_2$/3TFA]

Mn	-0.57744400	-2.56262500	-1.74224200
O	-0.38284400	-3.96922400	-0.87324000
O	-2.12082000	-2.32458200	-2.02904000
O	-0.02402700	-1.43438900	-0.62841000

O	0.39479900	-2.56724400	-2.98824200
Sc	-0.57352700	0.09308100	0.48585900
O	-1.94533800	1.58512400	0.21645100
O	0.59692100	-0.04181600	2.13496200
S	-3.33928300	1.84889400	-0.37890200
S	2.07410500	-0.46813700	2.31580100
O	-4.25026000	0.71076400	-0.16726900
O	-3.80686300	3.20133400	-0.07871500
O	2.69240500	-0.78749500	1.02135200
O	2.23259400	-1.38986900	3.44017900
C	-2.91667500	1.81905800	-2.21545100
C	2.83940500	1.16309100	2.86929400
F	2.73273400	2.06849300	1.89262100
F	4.12355600	0.96264800	3.13754400
F	2.22023000	1.61426200	3.95215200
F	-2.04156300	2.78067300	-2.49488300
F	-2.37473200	0.63630200	-2.52177900
F	-4.01925000	1.99612200	-2.93181900
C	-4.38701300	-1.40076800	2.12995100
C	-3.36292700	-1.51967700	0.97009200
O	-3.79917000	-2.18624100	-0.03160600
H	-3.14002400	-2.25836100	-0.79440000
O	-2.23552500	-1.06076800	1.12523900
F	-5.63826200	-1.37479500	1.68411700
F	-4.14967800	-0.30380900	2.84375800
F	-4.23839700	-2.47172300	2.92958800
C	4.72286400	-1.17521300	-1.26169100
C	3.30098400	-1.28197800	-1.87617800
O	2.93809700	-2.51300800	-2.06605200
H	2.03923300	-2.56219200	-2.49453800
O	2.66772800	-0.29512900	-2.19520600
F	4.93592200	-2.08787000	-0.31830900
F	4.91782600	0.04131000	-0.75433800
F	5.61968200	-1.36858200	-2.24653400
C	1.21605300	3.74831400	-0.40569900
C	1.55811300	2.28341200	-0.79368400
O	2.59634900	2.16129800	-1.52882100
H	2.74650700	1.18687600	-1.79664200
O	0.83252700	1.37154900	-0.41937800
F	0.50482100	3.76870700	0.71904400
F	0.48424000	4.28795600	-1.38973100
F	2.31833700	4.47645400	-0.23873100
C	0.78588700	-3.70055000	1.35968600
H	0.17164300	-3.79565700	0.25927800
H	0.89028100	-4.75900000	1.61327100
H	1.71148600	-3.18925900	1.08920800
H	0.11194300	-3.13550900	2.00660900

INT2[Sc(OTf)$_2$/3TFA]

Mn	-1.74210700	-2.58143700	1.18106800
O	-1.74396700	-4.00006700	0.19304500
O	-0.43218000	-2.55640800	2.07060500
O	-1.63215200	-1.43259800	-0.03998900
O	-3.13304300	-2.44147600	1.91878800
Sc	-0.13256000	-0.23880500	-0.67589500
O	0.61300100	0.14350800	1.12768200

O	1.38619300	0.58469700	-1.78011800
S	2.92768200	0.50970400	-1.77340800
S	0.26730200	1.00607300	2.37091400
O	3.42762000	-0.32330100	-0.66683100
O	3.46354900	0.30718700	-3.12157000
O	-0.70530500	0.34695200	3.24217900
O	0.04693500	2.40944700	1.99094800
C	1.92813000	0.92675000	3.25661400
C	3.35542800	2.28086500	-1.30017400
F	1.82509300	1.59297000	4.40197900
F	2.23409400	-0.34252900	3.50527500
F	2.87296900	1.47425400	2.50532100
F	2.86976100	3.12189100	-2.20951700
F	2.84128700	2.56746400	-0.10993600
F	4.67966700	2.40255300	-1.25093700
C	3.03633200	-3.39057800	-1.00105000
C	1.90374500	-2.69872900	-0.19654900
O	1.94536600	-2.96254500	1.05863700
H	1.09628500	-2.69116600	1.52963400
O	1.04369600	-2.04810000	-0.77912400
F	4.21202800	-3.25862000	-0.39502100
F	3.10907400	-2.89887700	-2.23191200
F	2.74206100	-4.70066500	-1.08280300
C	-4.76166600	0.26539300	-1.51792700
C	-4.43752800	-0.23926300	-0.08609300
O	-4.77579600	-1.48074000	0.06723100
H	-4.37051800	-1.86274200	0.89507900
O	-3.90056600	0.47146400	0.74030400
F	-3.92752800	-0.32912700	-2.38942000
F	-4.57840500	1.58392700	-1.59766200
F	-6.01456700	-0.02181700	-1.86516600
C	-0.94966700	3.95305800	-0.49629400
C	-1.66002800	2.60878700	-0.18633100
O	-2.74140100	2.73831300	0.47479100
H	-3.24022600	1.85525900	0.58757100
O	-1.21352400	1.55949100	-0.65285100
F	0.33196500	3.75509800	-0.77391000
F	-1.06202500	4.81152600	0.51094200
F	-1.54617000	4.48318100	-1.58023500
C	-1.72307800	-3.24494300	-2.59925600
H	-1.74128100	-3.75913200	-0.77554400
H	-2.14082200	-4.23061900	-2.80157700
H	-2.38241500	-2.37982600	-2.58444400
H	-0.64549400	-3.09906100	-2.66414200

[MnO_4/Sc(OTf)$_2$/3TFA]′

Mn	0.26646600	-2.90253000	-0.08122800
O	1.24364100	-3.63761500	-1.08593200
O	1.11870300	-1.94130200	0.89064100
O	-0.64765600	-1.82705200	-0.87004900
O	-0.61142400	-3.94229000	0.69878100
Sc	0.44531300	-0.04144000	-0.09128700
O	1.96056200	0.80240900	0.93491800
O	-0.65763000	1.14765300	-1.27515000
S	3.49351800	0.67005600	1.09296300
S	-2.10183000	1.65048100	-1.50502100

O	4.03223300	-0.40596000	0.24274600
O	4.14557100	1.97844000	1.09144600
O	-2.87973700	1.62263200	-0.25451600
O	-2.68513000	1.09081900	-2.72258900
C	3.59022800	0.02639400	2.86117200
C	-1.74636200	3.46552300	-1.86471900
F	-1.13373500	4.02160200	-0.82535900
F	-2.89941900	4.08802500	-2.08678200
F	-0.97292400	3.56432300	-2.94079800
F	3.02660300	0.90269000	3.68677300
F	2.95737600	-1.13863100	2.95438400
F	4.86808300	-0.13492600	3.18825700
C	3.84258500	0.07824900	-2.81618500
C	2.84425100	-0.89923600	-2.13950800
O	3.18876500	-2.13310900	-2.23765600
H	2.50892300	-2.74949300	-1.85111500
O	1.80467600	-0.47011600	-1.65687800
F	5.09889500	-0.32778300	-2.67468200
F	3.70695100	1.29792700	-2.30685500
F	3.54858900	0.12410100	-4.12577700
C	-4.73340200	-1.80423800	-0.27835600
C	-3.58634100	-2.55150100	0.45386900
O	-3.28079900	-3.67085600	-0.13881400
H	-2.48932000	-4.07633100	0.27818900
O	-3.04766800	-2.10373800	1.44438300
F	-4.27658200	-1.32446300	-1.43898700
F	-5.16281900	-0.79047300	0.46986400
F	-5.75595300	-2.62738000	-0.52365600
C	-1.60685100	2.22488900	2.55066900
C	-1.83745300	0.77123600	2.05608900
O	-2.94575200	0.26605300	2.43237300
H	-3.07066900	-0.67686000	2.07860000
O	-0.95206700	0.18499500	1.43420700
F	-0.70097200	2.83291300	1.78916600
F	-1.14012700	2.16678700	3.80834000
F	-2.73278900	2.92884200	2.54539300

INT1′[Sc(OTf)$_2$/3TFA]

Mn	-0.24893500	-1.44678600	-2.27258600
O	-1.22501300	-2.68199700	-2.45372300
O	-1.10982700	-0.11138100	-1.97710200
O	0.57956800	-1.60232100	-0.90281800
O	0.71588000	-1.31014600	-3.50433800
Sc	-0.59347100	0.00320500	0.17480300
O	-2.12204500	1.30131200	0.38381400
O	0.60446200	-0.55263800	1.70095400
S	-3.63056800	1.40659600	0.06129900
S	2.10447500	-0.92765200	1.81236200
O	-4.15003400	0.14817300	-0.50230900
O	-4.36363300	2.06410200	1.14159800
O	2.89315000	-0.27787300	0.75464800
O	2.29328100	-2.35279100	2.07846500
C	-3.57709600	2.63089800	-1.37061700
C	2.52949000	-0.01251900	3.40174700
F	2.28996200	1.28791800	3.24544900
F	3.81780600	-0.19612700	3.66880300

F	1.79528200	-0.47964100	4.40490100
F	-3.03355700	3.77271300	-0.96018500
F	-2.85264100	2.13089700	-2.36698200
F	-4.81723900	2.85400600	-1.79158700
C	-4.07838600	-2.28041700	1.43510200
C	-3.02209200	-2.17634800	0.30303600
O	-3.31989600	-2.86283400	-0.74113300
H	-2.59693800	-2.84211200	-1.42573900
O	-1.98441200	-1.55593300	0.49238500
F	-5.31322200	-2.33585600	0.95103100
F	-3.96795000	-1.24578900	2.26125900
F	-3.83236900	-3.40796400	2.12205800
C	5.06541100	-0.61276000	-1.42296600
C	3.67729900	-0.58137400	-2.11757800
O	3.37004200	-1.73409200	-2.64006800
H	2.50229400	-1.68048500	-3.10169900
O	3.01010800	0.42844700	-2.20016300
F	5.18510300	-1.65767400	-0.60794100
F	5.26504400	0.51066700	-0.73957200
F	6.01200100	-0.70522600	-2.37311700
C	1.19827000	3.66080800	0.65837000
C	1.54993600	2.43306800	-0.22759900
O	2.69360300	2.51779200	-0.78357000
H	2.91779000	1.69252300	-1.34061300
O	0.75115400	1.50822500	-0.34462300
F	0.04422100	3.45763800	1.28709300
F	1.08985100	4.74983800	-0.10969800
F	2.15883000	3.86274200	1.56211900
C	-0.34429300	-4.38734200	0.60840800
H	-0.50434700	-4.10851100	-0.44112300
H	-1.31159400	-4.51216200	1.11101900
H	0.20564700	-5.33535400	0.64353100
H	0.23844100	-3.61038400	1.11361300

TS1′[Sc(OTf)$_2$/3TFA]

Mn	-0.25668200	-1.85968900	-1.96930400
O	-0.96524500	-3.31004900	-1.45139200
O	-1.31273600	-0.64377200	-1.88922300
O	0.67030400	-1.51033500	-0.65507900
O	0.63876600	-2.06755500	-3.24490300
Sc	-0.59712200	0.06931000	0.08910400
O	-2.14579700	1.39901100	0.06939000
O	0.58741100	-0.04093500	1.73656700
S	-3.65882000	1.38136100	-0.22801800
S	2.08098300	-0.39796200	1.90820200
O	-4.14826600	0.01250800	-0.47494100
O	-4.39919300	2.24738200	0.68960800
O	2.90352400	0.21706000	0.85396600
O	2.27753600	-1.81318900	2.23220600
C	-3.69119100	2.24168400	-1.90377400
C	2.45324800	0.57226500	3.47687600
F	2.23886400	1.86763500	3.26410900
F	3.72785300	0.38193200	3.80338700
F	1.67400200	0.15088200	4.46750600
F	-3.17592100	3.46279700	-1.79023900
F	-2.98237000	1.54551400	-2.78735800

F	-4.95154700	2.32934100	-2.31826500
C	-4.05358700	-1.90183000	1.90298400
C	-2.95590700	-2.03800400	0.81475000
O	-3.20507400	-2.94961500	-0.05517300
H	-2.43048700	-3.09735400	-0.67596300
O	-1.92723100	-1.37841900	0.90135000
F	-5.26950100	-2.09667300	1.40615100
F	-3.99099800	-0.70674300	2.47916400
F	-3.81669300	-2.84009600	2.83682700
C	4.94177300	-0.83809400	-1.40960000
C	3.56125700	-0.93685800	-2.11395000
O	3.24777200	-2.17008700	-2.38280300
H	2.36124200	-2.22089400	-2.81974900
O	2.90358300	0.04199200	-2.40212100
F	5.00190800	-1.64096300	-0.34809700
F	5.18055600	0.41447600	-1.03175600
F	5.89803900	-1.21002300	-2.27716000
C	1.38678500	3.59149700	0.23661700
C	1.59296000	2.33843200	-0.66030400
O	2.70043800	2.33542800	-1.29236800
H	2.85378300	1.46078100	-1.79034400
O	0.70874000	1.48977100	-0.73715700
F	0.47546100	3.33933800	1.17424900
F	0.95040600	4.60226800	-0.52779500
F	2.52515400	3.95487200	0.82233400
C	0.25916500	-4.20025400	0.63724300
H	-0.32276600	-3.74582100	-0.35623500
H	-0.55630600	-4.71131300	1.15829400
H	0.98879000	-4.86546200	0.16699600
H	0.69756400	-3.35519900	1.16951700

INT2′[Sc(OTf)$_2$/3TFA]

Mn	-0.21691100	-2.92181300	-0.83187500
O	-1.18641500	-3.91158100	0.35999100
O	-1.06321200	-1.60351800	-1.25847000
O	0.75726900	-1.96812500	0.39714700
O	0.76372200	-3.76006100	-1.70129400
Sc	-0.44438700	-0.14089100	0.16388300
O	-1.88877800	1.13871700	-0.48932200
O	0.69720000	0.66653200	1.63890700
S	-3.36200300	1.05187100	-0.92797300
S	2.07104500	1.29747900	1.93422400
O	-3.94167800	-0.26755400	-0.61854200
O	-4.10771500	2.25896700	-0.56927700
O	2.75089500	1.73220200	0.70272900
O	2.82211700	0.51328900	2.91712100
C	-3.15943300	1.10471000	-2.80084300
C	1.51740000	2.86883500	2.81258500
F	0.74649400	3.58897300	2.00461600
F	2.59235700	3.57569900	3.14792300
F	0.83527500	2.55195100	3.90910700
F	-2.55396100	2.23653200	-3.15196800
F	-2.42935500	0.07212400	-3.21245900
F	-4.36077700	1.05017800	-3.36928000
C	-4.07972900	-0.85920400	2.40474600
C	-2.94753200	-1.55587900	1.60348100

O	-3.23272300	-2.73356000	1.21366800
H	-2.41365000	-3.23938900	0.79990600
O	-1.86148100	-0.98229400	1.48983800
F	-5.28531200	-1.21296000	1.97334900
F	-3.95597200	0.46357500	2.34348300
F	-3.95948900	-1.23746100	3.69158000
C	4.71177900	-1.49692200	-0.31927800
C	3.59622000	-2.08992000	-1.22106300
O	3.34566500	-3.33132700	-0.91440800
H	2.55379800	-3.66196000	-1.40064800
O	3.03946100	-1.43875200	-2.07879400
F	4.27856000	-1.44412700	0.94573000
F	5.01918900	-0.26654600	-0.72080200
F	5.80974000	-2.25710000	-0.36502800
C	1.28886300	2.90355500	-1.83877700
C	1.67213200	1.40173500	-1.77119000
O	2.77968900	1.12316300	-2.34727200
H	2.98322900	0.13435900	-2.28818400
O	0.90173700	0.58961900	-1.27117900
F	0.40879000	3.19784500	-0.88789100
F	0.72047000	3.13361200	-3.03449200
F	2.35383800	3.68951500	-1.71540300
C	1.16271600	-2.49618700	1.66480000
H	-0.71258700	-4.14207100	1.17298700
H	0.30363600	-2.62003100	2.33711500
H	1.68388000	-3.44987900	1.52346200
H	1.85279700	-1.77295800	2.11099700

[MnO_4/$Sc(OTf)_2$/TFA]

Mn	1.37625500	2.98872700	0.84070700
O	1.17714000	2.76704900	-0.75864400
O	0.55031700	4.19304600	1.36672100
O	0.76366200	1.54360400	1.38268900
O	2.87233000	3.15719700	1.21485700
O	1.72925100	-0.34442700	-1.47801000
O	-1.52633000	1.06913400	-1.21997800
S	-2.95809800	0.97802700	-0.62340400
S	3.22967300	-0.70272200	-1.25817100
O	-2.92862500	0.45646800	0.75279400
O	-3.73525400	2.17879900	-0.91998500
O	3.84892800	0.18981400	-0.27284800
O	3.89253100	-0.96528000	-2.53402800
C	3.02321300	-2.37078800	-0.40306200
C	-3.65581900	-0.40853200	-1.69203400
F	4.22478600	-2.87047400	-0.13994100
F	2.35218300	-2.20511600	0.73688200
F	2.35424000	-3.20611200	-1.18948000
F	-3.69271500	-0.02246300	-2.96198000
F	-2.88598700	-1.48653300	-1.57703000
F	-4.88421100	-0.69175000	-1.27462400
C	-1.63272200	-2.25706300	2.07397400
C	-0.81051700	-0.98294500	1.74683000
O	-0.64204300	-0.20941900	2.75966000
H	-0.08966800	0.57829700	2.51014300
O	-0.34468100	-0.83069000	0.62105100
Sc	0.35360300	0.77750500	-0.58091900

F	-2.10482100	-2.80151900	0.95989200
F	-2.64276700	-1.97425200	2.89170700
F	-0.81963200	-3.13682100	2.67770500

[MnO_3/Sc(OTf)$_2$/TFA]

Mn	1.20775500	3.10480700	1.12266700
O	1.11098600	2.93007200	-0.51466400
O	0.60348700	1.56453200	1.50156300
O	0.69269800	4.36218900	1.84930800
O	1.84827100	0.01235100	-1.39477200
O	-1.60008600	1.10921600	-1.09002600
S	-3.00961400	0.87090200	-0.50005100
S	3.36308800	-0.20067300	-1.16260500
O	-2.94608400	0.20598300	0.81194100
O	-3.86628800	2.04569100	-0.66099300
O	3.86310600	0.62695800	-0.05601900
O	4.09567700	-0.23343700	-2.42871100
C	3.34067500	-1.96970900	-0.51405300
C	-3.64196600	-0.42897500	-1.70645900
F	4.59073500	-2.36624800	-0.29734900
F	2.65794800	-2.01811000	0.62970300
F	2.76737700	-2.77410400	-1.40281900
F	-3.69760100	0.08093500	-2.93285600
F	-2.82525100	-1.47888900	-1.70037100
F	-4.85787100	-0.81087400	-1.32885100
C	-1.33225000	-2.51648600	1.86393300
C	-0.65046800	-1.14627300	1.61505600
O	-0.55248600	-0.41642100	2.66849200
H	-0.10231500	0.45447500	2.43754900
O	-0.21863000	-0.88200400	0.49653500
Sc	0.32903100	0.96827900	-0.47834900
F	-1.79782600	-3.01629600	0.72455800
F	-2.33165700	-2.40573800	2.73618800
F	-0.41673700	-3.36229400	2.36418500

INT1[Sc(OTf)$_2$/TFA]

Mn	1.41868000	2.90258500	0.95238300
O	1.48873000	2.49763700	-0.61898500
O	0.63755200	4.22435200	1.17997600
O	0.57944200	1.58590700	1.51551100
O	2.83808000	2.99484400	1.57581800
C	4.49125200	2.08570000	-1.38947000
H	4.22398200	1.70055900	-0.39850000
O	1.69974700	-0.64598300	-1.23494500
O	-1.31754400	1.05468400	-1.26361700
S	-2.81935800	1.19109300	-0.88464500
S	3.03935300	-1.29640700	-0.77455600
O	-3.06145900	0.74324600	0.49568600
O	-3.36517900	2.46956000	-1.33249100
O	3.47081200	-0.73773300	0.51256800
O	3.98109900	-1.40884800	-1.88521100
C	2.42612800	-3.04261800	-0.41250600
C	-3.54097300	-0.14302200	-2.00250600
F	3.45180400	-3.77988800	-0.00181700
F	1.49875700	-3.00071000	0.54234800
F	1.90443700	-3.57707500	-1.51097600

F	-3.32242600	0.16944400	-3.27422800
F	-2.96704700	-1.30958900	-1.72530800
F	-4.84729600	-0.22417600	-1.77961000
C	-2.23737100	-1.92894900	2.17307100
C	-1.23977000	-0.77772300	1.87874800
O	-1.14612000	0.07953400	2.83195900
H	-0.48929600	0.78878400	2.60237200
O	-0.59242100	-0.78963200	0.83501700
Sc	0.42086900	0.63012600	-0.38860900
H	5.52287500	1.79525400	-1.62201100
H	3.81542200	1.66032500	-2.14087000
H	4.40101200	3.17902500	-1.39389800
F	-2.62082600	-2.50579600	1.04087300
F	-3.30502200	-1.48052300	2.82628900
F	-1.61423400	-2.84025000	2.93543200

INT2[Sc(OTf)$_2$/TFA]

Mn	1.80202000	2.48732500	0.30913400
O	1.62692500	2.00061500	-1.25737700
O	1.24851400	3.91609200	0.52360700
O	0.73093200	1.33310600	0.91749100
O	3.37720800	2.19610000	0.88519500
C	4.57041100	4.55285700	2.03423700
H	3.81316900	3.00681200	1.29049200
O	1.30731000	-1.09210000	-1.68607600
O	-1.57921300	1.16154100	-1.37632500
S	-2.84639700	1.55668400	-0.57875000
S	2.73626800	-1.64310700	-1.45526100
O	-2.68471300	1.26873400	0.85490800
O	-3.36155500	2.85915400	-0.99897800
O	3.56194900	-0.68574300	-0.71002400
O	3.26150200	-2.27814400	-2.66427000
C	2.35396300	-3.03967800	-0.24841300
C	-4.05188800	0.26355500	-1.22937000
F	3.47757900	-3.69075000	0.03239800
F	1.84845500	-2.53024900	0.87731700
F	1.47390300	-3.88079300	-0.78110600
F	-4.19532800	0.39570100	-2.54391100
F	-3.58945600	-0.95456200	-0.95540000
F	-5.22787200	0.43402900	-0.63422500
C	-1.93140300	-2.06606400	2.19968000
C	-0.99535800	-0.96303400	1.63923000
O	-0.57289000	-0.15391700	2.54331400
H	-0.00176900	0.56324700	2.12922800
O	-0.71882000	-0.94775600	0.44389500
Sc	0.24761700	0.43897700	-0.90466700
H	3.79278300	4.69921900	2.78395200
H	5.48388100	4.02285400	2.30451600
H	4.54075400	5.13582900	1.11365400
F	-2.35995200	-2.85378200	1.22031300
F	-2.98253800	-1.50818600	2.80439100
F	-1.26354300	-2.80631000	3.09321400

INT3[Sc(OTf)$_2$/TFA]

Mn	-1.53345800	3.05093500	0.20250400
O	-0.93714100	2.72887500	-1.29474600

O	-3.22234400	2.86084100	0.27702100
O	-0.89229700	1.62995800	0.88302900
O	-0.79538400	4.32255100	1.11626300
H	-0.94323900	5.21873000	0.76438500
O	1.89905500	1.07639400	-1.33368600
O	-1.53798400	-0.36257200	-1.51396300
S	-2.65282900	-1.18483100	-0.82928700
S	3.19088700	1.19512000	-0.48973800
O	-2.55042400	-1.11794800	0.63744700
O	-3.95235500	-0.96476200	-1.46544700
O	2.90345900	1.11382300	0.94981700
O	4.06330300	2.25857300	-0.99141100
C	4.03189100	-0.42980900	-0.93884400
C	-2.10999600	-2.92550200	-1.30169000
F	5.18719900	-0.51051300	-0.28434800
F	3.25591600	-1.45343900	-0.59159100
F	4.26194700	-0.47688600	-2.24847200
F	-2.07260500	-3.04695600	-2.62514800
F	-0.89992000	-3.16819000	-0.80232300
F	-2.97789200	-3.79889300	-0.80043600
C	0.85861100	-2.20526800	2.39778700
C	0.33846400	-0.89291600	1.75559500
O	-0.22891900	-0.10755900	2.59879500
H	-0.57997100	0.71072700	2.11816800
O	0.49433900	-0.70059400	0.55488600
Sc	-0.06766200	0.86375700	-0.83295300
F	1.43324700	-2.97712800	1.48233700
F	-0.16013900	-2.87230400	2.95178900
F	1.75256300	-1.92098000	3.35126300
C	-3.93756900	2.10095600	1.24882600
H	-3.85866000	2.57427700	2.23684600
H	-4.98516800	2.08475800	0.92054700
H	-3.54222700	1.07679000	1.28215000

TS1[Sc(OTf)$_2$/TFA]

Mn	-1.13174300	-2.76752600	1.06629300
O	-1.17228400	-2.53917000	-0.57987000
O	-0.31339500	-4.03543100	1.41402100
O	-0.47907100	-1.28009800	1.43609000
O	-2.72361100	-2.92817500	1.45264200
C	-4.32219100	-2.81713300	-0.55219300
H	-3.54699200	-2.82594000	0.40532200
O	-1.80816200	0.46865600	-1.34488000
O	1.46213800	-1.04940100	-1.46801600
S	2.82674900	-1.34329300	-0.79341700
S	-3.15903000	0.95147500	-0.75197600
O	2.73917300	-1.10734400	0.65827400
O	3.43210300	-2.57627900	-1.29204000
O	-3.31074500	0.51005800	0.64123300
O	-4.25697400	0.74518300	-1.69745500
C	-2.83985800	2.80739400	-0.68682800
C	3.84696500	0.07822600	-1.49341800
F	-3.91249400	3.40831400	-0.18323000
F	-1.78813100	3.05031400	0.09227900
F	-2.60151900	3.27109000	-1.90836000
F	3.90585500	-0.01601700	-2.81689600

F	3.28535800	1.23843700	-1.15767200
F	5.07325800	0.01795300	-0.98659100
C	1.98667400	2.49261600	1.78915300
C	1.11023200	1.23229300	1.55947600
O	0.99984600	0.49371400	2.60462500
H	0.46831400	-0.32689500	2.38949100
O	0.61946100	1.02550000	0.45395600
Sc	-0.31022800	-0.63498200	-0.57018800
H	-5.24884200	-3.14422800	-0.07059000
H	-4.32197200	-1.77771600	-0.88723900
H	-3.89399900	-3.52873700	-1.26239400
F	1.86038200	3.33532100	0.77006200
F	3.26692600	2.11828400	1.89013500
F	1.62920800	3.11155900	2.91611400

TS2[Sc(OTf)$_2$/TFA]

Mn	2.12970300	2.43603400	0.10351500
O	1.86983100	1.77716700	-1.37187800
O	1.79422500	3.94166200	0.28587600
O	1.05538700	1.45054400	0.95177500
O	3.71765400	2.15022800	0.71148100
C	4.18644900	5.21672300	1.06054200
H	4.19361700	3.00664500	0.79575500
O	1.35005300	-1.35238700	-1.38169700
O	-1.28078700	1.06135600	-1.40744100
S	-2.64839800	1.54363700	-0.86227900
S	2.58425700	-2.17972500	-0.93505100
O	-2.74724300	1.36034300	0.59491700
O	-3.03316900	2.82646800	-1.44847900
O	3.25608900	-1.55022700	0.20888700
O	3.36840800	-2.62772800	-2.08595200
C	1.71215100	-3.70809400	-0.25982600
C	-3.77165800	0.23676900	-1.62295500
F	2.62655500	-4.55996800	0.19346400
F	0.89994900	-3.35947000	0.73601900
F	1.00351800	-4.28906900	-1.22288900
F	-3.74136800	0.33075800	-2.94803400
F	-3.35959300	-0.97333200	-1.25486500
F	-5.01255400	0.43372100	-1.19089600
C	-2.21389200	-1.16597900	2.58742300
C	-1.05862100	-0.35859200	1.94078400
O	-0.59470900	0.57390400	2.69053100
H	0.14495900	1.06332300	2.21138800
O	-0.64224000	-0.68679800	0.83122800
Sc	0.45700400	0.31822000	-0.71303000
H	3.69018600	5.22975900	2.02909400
H	5.19399600	4.80654600	0.97295100
H	3.75622400	5.76100000	0.22298900
F	-1.68008800	-2.08396800	3.40935600
F	-2.92326200	-1.78972100	1.65361300
F	-3.01615200	-0.37501000	3.29546400

TS3[Sc(OTf)$_2$/TFA]

Mn	-1.15963700	3.06813800	0.16725300
O	-0.85814800	2.77751500	-1.40739600
O	-2.94360600	3.25057700	0.69571300

O	-0.51713300	1.66221500	0.84592100
O	-1.11570700	4.52907500	0.96227800
H	-2.31869500	4.19764200	1.15934100
O	1.92908700	1.03418000	-1.26306600
O	-1.76609600	-0.25528000	-1.37219100
S	-2.80900700	-1.02580500	-0.53150100
S	3.17166000	1.08641900	-0.34016500
O	-2.41461600	-1.10504800	0.88296800
O	-4.17299200	-0.61132700	-0.86647500
O	2.80739600	0.83493100	1.06170500
O	4.03451700	2.22092200	-0.66983100
C	4.07547700	-0.45889900	-0.92627000
C	-2.58222700	-2.75989500	-1.22940700
F	5.19874000	-0.59235500	-0.22875000
F	3.30631700	-1.52874600	-0.73514400
F	4.36596800	-0.35166800	-2.21953700
F	-2.83627700	-2.76161200	-2.53425700
F	-1.33060300	-3.16304100	-1.02240900
F	-3.42096200	-3.58528900	-0.61220100
C	0.97188800	-2.43541800	2.01881600
C	0.48872300	-1.06016500	1.49089300
O	0.14752100	-0.24892800	2.42362400
H	-0.16348300	0.61952500	2.02121000
O	0.47138600	-0.84789700	0.28242000
Sc	-0.06386600	0.79140700	-0.99235400
F	0.02808300	-2.98703700	2.78729000
F	2.07961600	-2.27102800	2.74999100
F	1.23954500	-3.25412600	1.00697500
C	-3.62757900	2.26687200	1.48736900
H	-4.55399100	2.73686600	1.84027300
H	-3.86484400	1.40450200	0.85867000
H	-3.01374000	1.96033600	2.34390000