Efficient Epoxidation of Electron Deficient Olefins with a Cationic Manganese Complex

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Synthesis and Characterization

Experimental

Anhydrous acetonitrile (Aldrich, MeCN) was stored over activated 3 Å sieves for 3 days prior to use. Anhydrous diethyl ether (Aldrich, Et₂O) used without further purifications. (*R,R*)-(+)-cyclohexane-1,2-diamine was resolved as the tartrate salt as previously described.¹ N,N'-dimethyl-N,N'-bis(2-pyridylmethyl)-(*R,R*)-(+)-cyclohexane-1,2-diamine (***R,R*-mcp**) and N,N'-dimethyl-N,N'-bis(2-pyridylmethyl)-ethane-1,2-diamine (**mep**) were synthesized as previously described.^{2,4} Mn^{II}(CF₃SO₃)₂ was synthesized from Mn(CO₃) and triflic acid (Aldrich) as described.⁵ This solid was recrystallized twice from MeCN/Et₂O and dried at 150° C for 5 hours under vacuum.

Synthesis of [Mn^{II}(***R,R*-mcp**)(CF₃SO₃)₂] (1):

Under an N₂ atmosphere, N,N'-dimethyl-N,N'-bis(2-pyridylmethyl)-(*R,R*)-(+)-cyclohexane-1,2-diamine (***R,R*-mcp**, 322 mg, 1 mmole) was dissolved in 3 mL of MeCN along with 353 mg of Mn^{II}(CF₃SO₃)₂ (0.99 mmole). Once a homogeneous solution was obtained with stirring (~10 min), Et₂O was carefully layered on the solution to induce crystallization over 12 hrs. The crystals were isolated by vacuum filtration, washed with cold Et₂O to yield 0.480 mg (71%) of a brown, hygroscopic crystalline powder. X-ray quality crystals were grown from an MeCN solution with Et₂O diffusion. Anal. Calc. for MnS₂F₆O₆N₄C₂₂H₂₈: C 39.00; H 4.17; N 8.27. Found: C 38.52; H 3.95; N 7.99. μ_{eff} = 5.6 BM (295 K, MeCN).

Synthesis of [Mn^{II}(**mep**)(CF₃SO₃)₂] (2):

Under an N₂ atmosphere, N,N'-dimethyl-N,N'-bis(2-pyridylmethyl)-ethane-1,2-diamine (**mep**, 268 mg, 1 mmole) was added to 3 mL of MeCN along with 353 mg of Mn^{II}(CF₃SO₃)₂ (0.99 mmole). Once a homogeneous solution was obtained by stirring (~10 min), Et₂O was carefully layered on the solution to induce crystallization over 12 hrs. The crystals were isolated by vacuum filtration, washed with cold Et₂O to yield 0.331 mg (53%) of a brown, hygroscopic crystalline powder. X-ray quality crystals were grown from an MeCN solution with Et₂O diffusion. Anal. Calc. for MnS₂F₆O₆N₄C₁₈H₂₂: C 34.68; H 3.56; N 8.99. Found: C 34.56; H 3.46; N 9.04. μ_{eff} = 5.7 BM (295 K, MeCN).

Figure S11. ORTEP drawing of $[\text{Mn}^{\text{II}}(\text{R,R-mcp})(\text{CF}_3\text{SO}_3)_2]$ (**1**) at 50% probability with atom numbering scheme. The hydrogen atoms have been excluded for clarity.

Figure S21. ORTEP drawing of $[\text{Mn}^{\text{II}}(\text{mep})(\text{CF}_3\text{SO}_3)_2]$ (**2**) at 50% probability with atom numbering scheme shown. The hydrogen atoms have been excluded for clarity.

Crystallographic Data of [Mn^{II}(*R,R*-mcp)(CF₃SO₃)₂]:

Data Collection

A pale brown rectangular plate crystal of MnS₂F₆O₆N₄C₂₂H₂₈ was mounted on a quartz fiber using Paratone N hydrocarbon oil. All measurements were made on a Bruker-Siemens SMART¹ CCD area detector with graphite monochromated Mo-K α radiation. Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the measured positions of 2230 reflections in the range $4^\circ < 2\theta < 49.42^\circ$, corresponded to a primitive monoclinic cell with dimensions:

$$a = 9.1024(5) \text{ \AA}$$

$$b = 9.7740(6) \text{ \AA} \quad \beta = 101.871(2)^\circ$$

$$c = 16.2918(8) \text{ \AA}$$

$$V = 1418.4(1) \text{ \AA}^3$$

For $Z = 2$ and F.W. = 677.53, the calculated density is 1.59 g/cm³. Based on the systematic absences of:

$$0k0: k \pm 2n$$

packing considerations, a statistical analysis of intensity distribution, and the successful solution and refinement of the structure, the space group was determined to be:

$$P2_1 \text{ (#4)}$$

The data were collected at a temperature of $-110 \pm 1^\circ \text{C}$ using the ω scan technique to a maximum 2θ value of 49.4° . Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3° , counted for a total of 10 seconds per frame.

Data Reduction

Data were integrated by the program SAINT² with box parameters of 1.6 X 0.6. Of the 6305 reflections that were collected, 2484 were unique ($R_{\text{int}} = 0.060$); equivalent reflections (not including Friedel mates) were merged. No decay correction was applied. The linear absorption coefficient, μ , for Mo-K α radiation is 7.0 cm⁻¹. Data were analyzed for agreement and possible absorption using SADABS³. A semi-empirical absorption correction based on 2123 reflections with $I > 10\sigma(I)$ was applied that resulted in transmission factors ranging from 0.864 to 0.985. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods⁴ and expanded using Fourier techniques⁵. The non-hydrogen atoms were refined anisotropically. Absolute configuration was assigned based on prior knowledge of the chirality of the ligand and was confirmed by refinement of the Flack parameter to within 3 esd's of zero. Hydrogen atoms were located by difference Fourier but were constrained via a riding model to idealized positions 0.95 Å from their parent atoms. The final cycle of full-matrix least-squares refinement⁶ on F^2 was based on 4192 observed reflections and 399 variable parameters and converged (largest parameter shift was less than 1% of its esd) with unweighted and weighted agreement factors of:

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o| = 0.045$$

$$wR_2 = [\Sigma (w (F_o^2 - F_c^2)^2) / \Sigma w(F_o^2)^2]^{1/2} = 0.108$$

The standard deviation of an observation of unit weight⁷ was 0.90. The weighting scheme was based on counting statistics. Plots of $\Sigma w (|F_o| - |F_c|)^2$ versus $|F_o|$, reflection order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.86 and -1.17 e⁻/Å³, respectively. Neutral atom scattering factors were taken from Cromer and Waber⁸. Anomalous dispersion effects were included in F_c ⁹; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley¹⁰. The values for the mass attenuation coefficients are those of Creagh and Hubbell¹¹. All calculations were performed using the CrystalStructure^{12,13} crystallographic software package.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	MnS ₂ F ₆ O ₆ N ₄ C ₂₂ H ₂₈
Formula Weight	677.53
Crystal Color, Habit	pale brown rectangular plate
Crystal Dimensions	0.24 X 0.16 X 0.09 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination (2 θ range)	2230 (4° < 2 θ < 49.42°)
Lattice Parameters	a = 9.1024(5) Å b = 9.7740(6) Å c = 16.2918(8) Å β = 101.871(2)° V = 1418.4(1) Å ³
Space Group	P2 ₁ (#4)
Z value	2
D _{calc}	1.586 g/cm ³
F ₀₀₀	694.00
μ (MoK α)	6.96 cm ⁻¹

B. Intensity Measurements

Diffractometer	Bruker-Siemens SMART CCD
Radiation	MoK α (λ = 0.71069 Å) graphite monochromated
Temperature	-110° C
Scan Type	ω (0.3°/frame)
Scan Rate	10 sec Frame Exposure
2 θ _{max}	49.4°
No. of Reflections Measured	Total: 6305 Unique: 2484 (R _{int} = 0.060)
Corrections	Absorption, Lorentz, polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELX97)
Refinement	Full-matrix least-squares on F ²
Function Minimized	$\sum w (F_o^2 - F_c^2)^2$
Least Squares Weights	$1/\sigma^2(F_o^2) = 1/\sigma^2(F_o)/(4F_o^2)$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I > 0.00 σ (I))	4192
No. Variables	399
Reflection/Parameter Ratio	10.51
Residuals: R ₁ ; wR ₂	0.045 ; 0.108
Goodness of Fit Indicator	0.90
Max Shift/Error in Final Cycle	0.00
Maximum peak in Final Diff. Map	0.86 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-1.17 e ⁻ /Å ³

Table S11. Atomic coordinates and B_{iso}/B_{eq} for [Mn^{II}(*R,R*-mcp)(CF₃SO₃)₂]:

atom	x	y	z	B _{eq}
Mn(1)	0.06437(9)	0.0618(1)	0.74708(5)	1.53(2)
S(1)	0.2134(2)	-0.1781(2)	0.88129(8)	1.95(3)
S(2)	0.3274(2)	0.0216(1)	0.62437(8)	1.85(3)
F(1)	0.0752(5)	-0.4156(4)	0.8700(3)	4.5(1)
F(2)	0.2494(5)	-0.4027(4)	0.7989(3)	4.7(1)
F(3)	0.3074(5)	-0.4198(4)	0.9330(3)	5.3(1)
F(4)	0.2651(4)	-0.2305(4)	0.6588(2)	3.24(9)
F(5)	0.4302(4)	-0.2110(4)	0.5826(2)	3.34(9)
F(6)	0.4914(4)	-0.1681(4)	0.7145(2)	3.60(9)
O(1)	0.0951(4)	-0.1365(4)	0.8107(2)	2.05(9)
O(2)	0.3608(4)	-0.1392(5)	0.8736(3)	3.0(1)
O(3)	0.1726(5)	-0.1593(4)	0.9614(2)	2.8(1)
O(4)	0.2667(4)	0.0630(4)	0.6976(2)	1.87(8)
O(5)	0.2157(4)	0.0109(4)	0.5478(2)	2.57(9)
O(6)	0.4638(4)	0.0895(4)	0.6191(3)	2.7(1)
N(1)	-0.1188(5)	0.1239(5)	0.8175(3)	1.6(1)
N(2)	0.1852(5)	0.1677(5)	0.8615(3)	1.6(1)
N(3)	-0.0468(5)	0.2414(5)	0.6663(3)	1.5(1)
N(4)	-0.0818(5)	-0.0380(5)	0.6394(3)	1.7(1)
C(1)	-0.2437(6)	0.0233(6)	0.8028(3)	2.4(1)
C(2)	-0.0470(6)	0.1202(6)	0.9079(3)	1.7(1)
C(3)	0.1077(6)	0.1786(6)	0.9241(3)	1.7(1)
C(4)	0.1752(7)	0.2321(7)	1.0017(4)	2.4(1)
C(5)	0.3233(7)	0.2746(7)	1.0167(4)	2.7(1)
C(6)	0.4016(7)	0.2634(7)	0.9525(4)	2.4(1)
C(7)	0.3288(6)	0.2111(6)	0.8766(4)	2.2(1)
C(8)	-0.1684(6)	0.2672(5)	0.7903(3)	1.7(1)
C(9)	-0.3100(6)	0.3122(6)	0.8199(4)	2.4(1)
C(10)	-0.3589(8)	0.4561(7)	0.7902(4)	3.3(2)
C(11)	0.0624(7)	0.3543(6)	0.6726(4)	2.3(1)
C(12)	-0.0843(7)	0.1892(6)	0.5789(4)	2.1(1)
C(13)	-0.1418(6)	0.0441(6)	0.5740(3)	1.6(1)
C(14)	-0.2466(6)	-0.0035(6)	0.5057(3)	2.0(1)
C(15)	-0.2857(7)	-0.1389(6)	0.5031(4)	2.3(1)
C(16)	-0.2227(7)	-0.2253(7)	0.5674(3)	2.3(1)
C(17)	-0.1226(6)	-0.1704(6)	0.6344(3)	2.4(1)
C(18)	-0.1891(6)	0.2791(6)	0.6945(3)	1.7(1)
C(19)	-0.2458(7)	0.4249(6)	0.6645(4)	2.6(1)
C(20)	-0.3895(8)	0.4620(7)	0.6949(4)	3.4(2)
C(21)	0.2097(8)	-0.3641(6)	0.8694(4)	3.0(2)
C(22)	0.3808(7)	-0.1567(6)	0.6470(4)	2.3(1)

Table S11. Atomic coordinates and B_{iso}/B_{eq} for [Mn^{II}(**R,R**-mcp)(CF₃SO₃)₂]: (continued)

atom	x	y	z	B _{eq}
H(1)	-0.1059(6)	0.1721(6)	0.9385(3)	2.1(1)
H(2)	-0.0420(6)	0.0280(6)	0.9266(3)	2.1(1)
H(3)	0.1186(7)	0.2399(7)	1.0444(4)	2.9(2)
H(4)	0.3697(7)	0.3110(7)	1.0698(4)	3.1(2)
H(5)	0.5037(7)	0.2910(7)	0.9607(4)	2.8(2)
H(6)	0.3820(6)	0.2036(6)	0.8323(4)	2.6(2)
H(7)	-0.0898(6)	0.3280(5)	0.8142(3)	1.9(1)
H(8)	-0.3886(6)	0.2508(6)	0.7968(4)	2.8(2)
H(9)	-0.2930(6)	0.3088(6)	0.8794(4)	2.8(2)
H(10)	-0.4464(8)	0.4810(7)	0.8099(4)	4.0(2)
H(11)	-0.2799(8)	0.5179(7)	0.8119(4)	4.0(2)
H(12)	-0.4664(8)	0.3984(7)	0.6726(4)	4.1(2)
H(13)	-0.4206(8)	0.5515(7)	0.6763(4)	4.1(2)
H(14)	-0.1700(7)	0.4890(6)	0.6876(4)	3.2(2)
H(15)	-0.2633(7)	0.4287(6)	0.6050(4)	3.2(2)
H(16)	-0.2642(6)	0.2151(6)	0.6704(3)	2.0(1)
H(17)	-0.3141(6)	0.0471(6)	0.8362(3)	2.9(2)
H(18)	-0.2919(6)	0.0245(6)	0.7453(3)	2.9(2)
H(19)	-0.2054(6)	-0.0657(6)	0.8177(3)	2.9(2)
H(20)	0.1509(7)	0.3221(6)	0.6565(4)	2.9(2)
H(21)	0.0201(7)	0.4267(6)	0.6365(4)	2.9(2)
H(22)	0.0868(7)	0.3866(6)	0.7288(4)	2.9(2)
H(23)	-0.1595(7)	0.2463(6)	0.5471(4)	2.5(2)
H(24)	0.0033(7)	0.1923(6)	0.5557(4)	2.5(2)
H(25)	-0.2892(6)	0.0569(6)	0.4615(3)	2.4(2)
H(26)	-0.3573(7)	-0.1734(6)	0.4569(4)	2.6(2)
H(27)	-0.2480(7)	-0.3197(7)	0.5659(3)	2.8(2)
H(28)	-0.0795(6)	-0.2287(6)	0.6796(3)	2.8(2)

$$B_{eq} = 8/3 \pi (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos \gamma + 2U_{13}(aa^*cc^*)\cos \beta + 2U_{23}(bb^*cc^*)\cos \alpha)$$

Table S12. Anisotropic Displacement Parameters for [Mn^{II}(*R,R*-mcp)(CF₃SO₃)₂]:

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Mn(1)	0.0227(4)	0.0197(5)	0.0146(4)	0.0007(4)	0.0010(3)	-0.0014(4)
S(1)	0.0307(9)	0.0216(8)	0.0196(8)	0.0012(7)	-0.0001(6)	0.0047(6)
S(2)	0.0275(8)	0.0229(9)	0.0212(7)	0.0028(7)	0.0082(6)	-0.0006(6)
F(1)	0.063(3)	0.032(3)	0.080(3)	-0.020(2)	0.023(2)	-0.007(2)
F(2)	0.092(3)	0.035(3)	0.056(3)	0.005(2)	0.029(2)	-0.015(2)
F(3)	0.090(3)	0.034(3)	0.062(3)	0.022(3)	-0.018(2)	0.018(2)
F(4)	0.049(2)	0.026(2)	0.051(2)	-0.013(2)	0.017(2)	-0.001(2)
F(5)	0.048(2)	0.032(2)	0.050(2)	0.005(2)	0.017(2)	-0.015(2)
F(6)	0.048(2)	0.033(2)	0.045(2)	0.011(2)	-0.015(2)	0.005(2)
O(1)	0.028(2)	0.030(2)	0.015(2)	0.001(2)	-0.007(2)	0.005(2)
O(2)	0.026(2)	0.038(3)	0.048(3)	-0.002(2)	-0.000(2)	0.012(2)
O(3)	0.058(3)	0.032(3)	0.020(2)	0.002(2)	0.014(2)	0.005(2)
O(4)	0.028(2)	0.022(2)	0.023(2)	0.005(2)	0.008(2)	-0.004(2)
O(5)	0.032(2)	0.046(3)	0.019(2)	0.007(2)	0.002(2)	0.002(2)
O(6)	0.034(2)	0.030(3)	0.041(2)	-0.005(2)	0.017(2)	-0.001(2)
N(1)	0.026(3)	0.017(3)	0.015(2)	-0.006(2)	-0.002(2)	-0.003(2)
N(2)	0.018(3)	0.023(3)	0.021(3)	-0.002(2)	0.007(2)	-0.003(2)
N(3)	0.022(3)	0.016(3)	0.018(2)	-0.002(2)	0.006(2)	-0.002(2)
N(4)	0.028(3)	0.016(3)	0.019(3)	0.002(2)	-0.001(2)	0.002(2)
C(1)	0.035(3)	0.033(4)	0.024(3)	-0.005(3)	0.006(3)	-0.001(3)
C(2)	0.022(3)	0.022(3)	0.021(3)	0.000(3)	0.002(3)	0.002(2)
C(3)	0.026(3)	0.018(3)	0.017(3)	0.002(3)	-0.000(3)	0.001(2)
C(4)	0.032(4)	0.035(4)	0.026(3)	-0.002(3)	0.005(3)	0.000(3)
C(5)	0.028(3)	0.048(4)	0.023(3)	-0.000(3)	-0.004(3)	-0.009(3)
C(6)	0.020(3)	0.035(4)	0.033(3)	-0.004(3)	-0.001(3)	-0.006(3)
C(7)	0.023(3)	0.031(4)	0.029(3)	-0.002(3)	0.004(3)	-0.003(3)
C(8)	0.025(3)	0.014(3)	0.022(3)	0.002(2)	-0.001(2)	0.002(2)
C(9)	0.024(3)	0.033(4)	0.032(3)	0.012(3)	0.006(3)	0.004(3)
C(10)	0.041(4)	0.042(4)	0.044(4)	0.020(4)	0.013(3)	-0.003(3)
C(11)	0.037(4)	0.022(4)	0.032(3)	-0.007(3)	0.017(3)	-0.005(3)
C(12)	0.031(4)	0.021(3)	0.028(3)	-0.000(3)	0.009(3)	-0.006(3)
C(13)	0.027(3)	0.018(3)	0.017(3)	0.005(3)	0.007(2)	0.003(3)
C(14)	0.034(4)	0.031(4)	0.010(3)	0.006(3)	-0.001(3)	0.001(3)
C(15)	0.033(4)	0.027(4)	0.021(3)	-0.006(3)	-0.005(3)	-0.008(3)
C(16)	0.040(4)	0.025(4)	0.023(3)	-0.006(3)	0.006(3)	-0.006(3)
C(17)	0.038(4)	0.024(4)	0.027(3)	-0.002(3)	0.004(3)	0.005(3)
C(18)	0.023(3)	0.020(3)	0.022(3)	0.003(3)	0.001(2)	0.001(2)
C(19)	0.049(4)	0.025(3)	0.027(3)	0.009(3)	0.012(3)	0.005(3)
C(20)	0.054(4)	0.038(4)	0.037(4)	0.025(4)	0.006(3)	0.003(3)
C(21)	0.053(5)	0.019(4)	0.038(4)	0.005(3)	0.004(4)	0.002(3)
C(22)	0.038(4)	0.016(3)	0.038(4)	0.011(3)	0.014(3)	-0.002(3)

The general temperature factor expression:

$$\exp(-2\pi^2(a^2U_{11}h^2 + b^2U_{22}k^2 + c^2U_{33}l^2 + 2a*b*U_{12}hk + 2a*c*U_{13}hl + 2b*c*U_{23}kl))$$

Table S13. Bond lengths (Å) for [Mn^{II}(*R,R*-mcp)(CF₃SO₃)₂]:

atom	atom	distance	atom	atom	distance
Mn(1)	O(1)	2.189(4)	Mn(1)	O(4)	2.157(3)
Mn(1)	N(1)	2.292(5)	Mn(1)	N(2)	2.216(4)
Mn(1)	N(3)	2.300(5)	Mn(1)	N(4)	2.199(4)
S(1)	O(1)	1.462(4)	S(1)	O(2)	1.424(4)
S(1)	O(3)	1.440(4)	S(1)	C(21)	1.828(6)
S(2)	O(4)	1.471(3)	S(2)	O(5)	1.441(4)
S(2)	O(6)	1.427(4)	S(2)	C(22)	1.826(6)
F(1)	C(21)	1.325(7)	F(2)	C(21)	1.328(7)
F(3)	C(21)	1.334(7)	F(4)	C(22)	1.323(7)
F(5)	C(22)	1.334(6)	F(6)	C(22)	1.334(6)
N(1)	C(1)	1.485(7)	N(1)	C(2)	1.483(6)
N(1)	C(8)	1.510(7)	N(2)	C(3)	1.359(7)
N(2)	C(7)	1.347(7)	N(3)	C(11)	1.475(7)
N(3)	C(12)	1.485(7)	N(3)	C(18)	1.506(6)
N(4)	C(13)	1.356(7)	N(4)	C(17)	1.344(8)
C(2)	C(3)	1.491(7)	C(3)	C(4)	1.390(8)
C(4)	C(5)	1.383(8)	C(5)	C(6)	1.385(8)
C(6)	C(7)	1.377(8)	C(8)	C(9)	1.531(7)
C(8)	C(18)	1.537(7)	C(9)	C(10)	1.524(9)
C(10)	C(20)	1.521(9)	C(12)	C(13)	1.508(8)
C(13)	C(14)	1.388(7)	C(14)	C(15)	1.370(8)
C(15)	C(16)	1.376(8)	C(16)	C(17)	1.378(7)
C(18)	C(19)	1.560(8)	C(19)	C(20)	1.534(9)

Table S14. Bond lengths involving hydrogens (Å) for [Mn^{II}(*R,R*-mcp)(CF₃SO₃)₂]:

atom	atom	distance	atom	atom	distance
C(1)	H(17)	0.950(8)	C(1)	H(18)	0.950(8)
C(1)	H(19)	0.950(8)	C(2)	H(1)	0.950(7)
C(2)	H(2)	0.95	C(4)	H(3)	0.950(8)
C(5)	H(4)	0.950(8)	C(6)	H(5)	0.950(8)
C(7)	H(6)	0.950(8)	C(8)	H(7)	0.950(7)
C(9)	H(8)	0.950(9)	C(9)	H(9)	0.950(9)
C(10)	H(10)	0.950(9)	C(10)	H(11)	0.950(9)
C(11)	H(20)	0.950(9)	C(11)	H(21)	0.950(9)
C(11)	H(22)	0.950(9)	C(12)	H(23)	0.950(8)
C(12)	H(24)	0.950(8)	C(14)	H(25)	0.950(8)
C(15)	H(26)	0.950(8)	C(16)	H(27)	0.95
C(17)	H(28)	0.95	C(18)	H(16)	0.950(8)
C(19)	H(14)	0.950(9)	C(19)	H(15)	0.950(9)
C(20)	H(12)	0.950(9)	C(20)	H(13)	0.950(9)

Table S15. Bond angles(°) for [Mn^{II}(*R,R*-mcp)(CF₃SO₃)₂]:

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Mn(1)	O(4)	98.4(2)	O(1)	Mn(1)	N(1)	91.9(2)
O(4)	Mn(1)	N(1)	161.9(2)	O(1)	Mn(1)	N(2)	91.3(2)
O(4)	Mn(1)	N(2)	89.9(2)	N(1)	Mn(1)	N(2)	75.0(2)
O(1)	Mn(1)	N(3)	160.9(1)	O(4)	Mn(1)	N(3)	95.2(2)
N(1)	Mn(1)	N(3)	78.7(2)	N(2)	Mn(1)	N(3)	102.0(2)
O(1)	Mn(1)	N(4)	89.0(2)	O(4)	Mn(1)	N(4)	97.3(2)
N(1)	Mn(1)	N(4)	97.7(2)	N(2)	Mn(1)	N(4)	172.7(2)
N(3)	Mn(1)	N(4)	76.1(2)	O(1)	S(1)	O(2)	114.3(3)
O(1)	S(1)	O(3)	113.1(3)	O(2)	S(1)	O(3)	117.9(3)
O(1)	S(1)	C(21)	101.5(3)	O(2)	S(1)	C(21)	104.7(3)
O(3)	S(1)	C(21)	102.7(3)	O(4)	S(2)	O(5)	113.9(2)
O(4)	S(2)	O(6)	113.4(2)	O(5)	S(2)	O(6)	116.7(2)
O(4)	S(2)	C(22)	103.2(3)	O(5)	S(2)	C(22)	102.6(3)
O(6)	S(2)	C(22)	104.9(3)	Mn(1)	O(1)	S(1)	128.3(2)
Mn(1)	O(4)	S(2)	142.5(2)	Mn(1)	N(1)	C(1)	110.9(3)
Mn(1)	N(1)	C(2)	105.8(3)	C(1)	N(1)	C(2)	108.1(4)
Mn(1)	N(1)	C(8)	107.6(3)	C(1)	N(1)	C(8)	113.2(4)
C(2)	N(1)	C(8)	111.0(4)	Mn(1)	N(2)	C(3)	115.0(4)
Mn(1)	N(2)	C(7)	126.5(4)	C(3)	N(2)	C(7)	118.2(5)
Mn(1)	N(3)	C(11)	108.7(3)	Mn(1)	N(3)	C(12)	105.9(3)
C(11)	N(3)	C(12)	110.0(4)	Mn(1)	N(3)	C(18)	108.5(3)
C(11)	N(3)	C(18)	113.9(4)	C(12)	N(3)	C(18)	109.5(4)
Mn(1)	N(4)	C(13)	116.4(4)	Mn(1)	N(4)	C(17)	126.1(4)
C(13)	N(4)	C(17)	117.4(5)	N(1)	C(2)	C(3)	112.0(4)
N(2)	C(3)	C(2)	117.0(5)	N(2)	C(3)	C(4)	120.8(5)
C(2)	C(3)	C(4)	122.0(5)	C(3)	C(4)	C(5)	120.4(6)
C(4)	C(5)	C(6)	118.5(5)	C(5)	C(6)	C(7)	118.7(6)
N(2)	C(7)	C(6)	123.4(6)	N(1)	C(8)	C(9)	113.2(5)
N(1)	C(8)	C(18)	109.6(4)	C(9)	C(8)	C(18)	111.3(4)
C(8)	C(9)	C(10)	112.0(5)	C(9)	C(10)	C(20)	109.9(5)
N(3)	C(12)	C(13)	112.5(5)	N(4)	C(13)	C(12)	115.8(5)
N(4)	C(13)	C(14)	122.1(5)	C(12)	C(13)	C(14)	122.1(5)
C(13)	C(14)	C(15)	118.7(5)	C(14)	C(15)	C(16)	120.3(6)
C(15)	C(16)	C(17)	118.0(6)	N(4)	C(17)	C(16)	123.5(6)
N(3)	C(18)	C(8)	111.0(4)	N(3)	C(18)	C(19)	112.2(5)
C(8)	C(18)	C(19)	110.5(5)	C(18)	C(19)	C(20)	111.4(5)
C(10)	C(20)	C(19)	109.3(5)	S(1)	C(21)	F(1)	112.0(5)
S(1)	C(21)	F(2)	111.8(4)	F(1)	C(21)	F(2)	108.3(6)
S(1)	C(21)	F(3)	109.2(5)	F(1)	C(21)	F(3)	108.0(5)
F(2)	C(21)	F(3)	107.4(6)	S(2)	C(22)	F(4)	111.3(4)
S(2)	C(22)	F(5)	109.8(4)	F(4)	C(22)	F(5)	107.7(5)
S(2)	C(22)	F(6)	111.8(4)	F(4)	C(22)	F(6)	108.9(5)
F(5)	C(22)	F(6)	107.2(5)				

Table S16. Bond angles involving hydrogens(°) for [Mn^{II}(*R,R*-mcp)(CF₃SO₃)₂]:

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	H(18)	109.5(3)	H(17)	C(1)	H(18)	109.5
N(1)	C(1)	H(19)	109.7(3)	H(17)	C(1)	H(19)	109.5
H(18)	C(1)	H(19)	109.5	N(1)	C(2)	H(1)	109.1(3)
C(3)	C(2)	H(1)	108.5(3)	N(1)	C(2)	H(2)	108.9(3)
C(3)	C(2)	H(2)	108.9(3)	H(1)	C(2)	H(2)	109.5
C(3)	C(4)	H(3)	119.5(3)	C(5)	C(4)	H(3)	120.1(4)
C(4)	C(5)	H(4)	120.5(4)	C(6)	C(5)	H(4)	121.0(4)
C(5)	C(6)	H(5)	120.8(3)	C(7)	C(6)	H(5)	120.5(4)
N(2)	C(7)	H(6)	117.6(3)	C(6)	C(7)	H(6)	119.0(4)
N(1)	C(8)	H(7)	107.8(3)	C(9)	C(8)	H(7)	107.6(3)
C(18)	C(8)	H(7)	107.1(3)	C(8)	C(9)	H(8)	107.9(3)
C(10)	C(9)	H(8)	108.1(4)	C(8)	C(9)	H(9)	109.9(3)
C(10)	C(9)	H(9)	109.4(3)	H(8)	C(9)	H(9)	109.5
C(9)	C(10)	H(10)	109.8(3)	C(20)	C(10)	H(10)	110.3(4)
C(9)	C(10)	H(11)	108.6(4)	C(20)	C(10)	H(11)	108.8(4)
H(10)	C(10)	H(11)	109.5(4)	N(3)	C(11)	H(20)	109.3(3)
N(3)	C(11)	H(21)	109.5(3)	H(20)	C(11)	H(21)	109.5(3)
N(3)	C(11)	H(22)	109.6(3)	H(20)	C(11)	H(22)	109.5
H(21)	C(11)	H(22)	109.5	N(3)	C(12)	H(23)	108.6(3)
C(13)	C(12)	H(23)	108.7(3)	N(3)	C(12)	H(24)	109.0(3)
C(13)	C(12)	H(24)	108.6(3)	H(23)	C(12)	H(24)	109.5
C(13)	C(14)	H(25)	120.3(3)	C(15)	C(14)	H(25)	120.9(3)
C(14)	C(15)	H(26)	119.9(3)	C(16)	C(15)	H(26)	119.8(4)
C(15)	C(16)	H(27)	121.0(4)	C(17)	C(16)	H(27)	121.0(4)
N(4)	C(17)	H(28)	117.8(3)	C(16)	C(17)	H(28)	118.7(4)
N(3)	C(18)	H(16)	107.7(3)	C(8)	C(18)	H(16)	107.3(3)
C(19)	C(18)	H(16)	108.0(3)	C(18)	C(19)	H(14)	108.2(3)
C(20)	C(19)	H(14)	108.3(4)	C(18)	C(19)	H(15)	109.3(3)
C(20)	C(19)	H(15)	110.2(3)	H(14)	C(19)	H(15)	109.5
C(10)	C(20)	H(12)	109.3(4)	C(19)	C(20)	H(12)	109.4(4)
C(10)	C(20)	H(13)	109.9(3)	C(19)	C(20)	H(13)	109.4(4)
H(12)	C(20)	H(13)	109.5				

Table S17. Torsion Angles (°) for [Mn^{II}(*R,R*-mcp)(CF₃SO₃)₂]:

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(4)	Mn(1)	O(1)	S(1)	63.9(7)	N(1)	Mn(1)	O(1)	S(1)	-101.3(7)
N(2)	Mn(1)	O(1)	S(1)	-26.2(8)	N(3)	Mn(1)	O(1)	S(1)	-161.0(1)
N(4)	Mn(1)	O(1)	S(1)	161.1(6)	O(1)	Mn(1)	O(4)	S(2)	89.2(9)
N(1)	Mn(1)	O(4)	S(2)	-146.8(1)	N(2)	Mn(1)	O(4)	S(2)	-179.5(8)
N(3)	Mn(1)	O(4)	S(2)	-77.5(9)	N(4)	Mn(1)	O(4)	S(2)	-0.8(1)
O(1)	Mn(1)	N(1)	C(1)	-57.4(7)	O(1)	Mn(1)	N(1)	C(2)	59.5(7)
O(1)	Mn(1)	N(1)	C(8)	178.3(6)	O(4)	Mn(1)	N(1)	C(1)	177.7(1)
O(4)	Mn(1)	N(1)	C(2)	-65.3(2)	O(4)	Mn(1)	N(1)	C(8)	53.4(2)
N(2)	Mn(1)	N(1)	C(1)	-148.3(7)	N(2)	Mn(1)	N(1)	C(2)	-31.3(6)
N(2)	Mn(1)	N(1)	C(8)	87.5(7)	N(3)	Mn(1)	N(1)	C(1)	105.9(7)
N(3)	Mn(1)	N(1)	C(2)	-137.2(7)	N(3)	Mn(1)	N(1)	C(8)	-18.4(7)
N(4)	Mn(1)	N(1)	C(1)	31.8(8)	N(4)	Mn(1)	N(1)	C(2)	148.8(7)
N(4)	Mn(1)	N(1)	C(8)	-92.5(7)	O(1)	Mn(1)	N(2)	C(3)	-73.3(7)
O(1)	Mn(1)	N(2)	C(7)	101.1(9)	O(4)	Mn(1)	N(2)	C(3)	-171.7(7)
O(4)	Mn(1)	N(2)	C(7)	2.7(9)	N(1)	Mn(1)	N(2)	C(3)	18.3(7)
N(1)	Mn(1)	N(2)	C(7)	-167.3(9)	N(3)	Mn(1)	N(2)	C(3)	93.0(8)
N(3)	Mn(1)	N(2)	C(7)	-92.6(9)	N(4)	Mn(1)	N(2)	C(3)	18.8(5)
N(4)	Mn(1)	N(2)	C(7)	-166.8(4)	O(1)	Mn(1)	N(3)	C(11)	175.8(1)
O(1)	Mn(1)	N(3)	C(12)	-66.1(2)	O(1)	Mn(1)	N(3)	C(18)	51.4(2)
O(4)	Mn(1)	N(3)	C(11)	-48.7(7)	O(4)	Mn(1)	N(3)	C(12)	69.4(7)
O(4)	Mn(1)	N(3)	C(18)	-173.1(6)	N(1)	Mn(1)	N(3)	C(11)	114.1(7)
N(1)	Mn(1)	N(3)	C(12)	-127.8(7)	N(1)	Mn(1)	N(3)	C(18)	-10.3(7)
N(2)	Mn(1)	N(3)	C(11)	42.3(8)	N(2)	Mn(1)	N(3)	C(12)	160.4(7)
N(2)	Mn(1)	N(3)	C(18)	-82.1(7)	N(4)	Mn(1)	N(3)	C(11)	-144.9(7)
N(4)	Mn(1)	N(3)	C(12)	-26.8(7)	N(4)	Mn(1)	N(3)	C(18)	90.7(7)
O(1)	Mn(1)	N(4)	C(13)	179.3(7)	O(1)	Mn(1)	N(4)	C(17)	2.8(9)
O(4)	Mn(1)	N(4)	C(13)	-82.4(8)	O(4)	Mn(1)	N(4)	C(17)	101.1(9)
N(1)	Mn(1)	N(4)	C(13)	87.5(8)	N(1)	Mn(1)	N(4)	C(17)	-89.0(9)
N(2)	Mn(1)	N(4)	C(13)	87.0(5)	N(2)	Mn(1)	N(4)	C(17)	-89.5(5)
N(3)	Mn(1)	N(4)	C(13)	11.2(7)	N(3)	Mn(1)	N(4)	C(17)	-165.3(9)
O(2)	S(1)	O(1)	Mn(1)	-45.4(7)	O(3)	S(1)	O(1)	Mn(1)	93.3(6)
C(21)	S(1)	O(1)	Mn(1)	-157.5(5)	O(1)	S(1)	C(21)	F(1)	-57.0(9)
O(1)	S(1)	C(21)	F(2)	64.8(9)	O(1)	S(1)	C(21)	F(3)	-176.6(7)
O(2)	S(1)	C(21)	F(1)	-176.2(8)	O(2)	S(1)	C(21)	F(2)	-54.4(1)
O(2)	S(1)	C(21)	F(3)	64.3(9)	O(3)	S(1)	C(21)	F(1)	60.1(9)
O(3)	S(1)	C(21)	F(2)	-178.1(8)	O(3)	S(1)	C(21)	F(3)	-59.4(9)
O(5)	S(2)	O(4)	Mn(1)	25.1(9)	O(6)	S(2)	O(4)	Mn(1)	161.8(5)

Table S17. Torsion angles (°) for [Mn^{II}(*R,R*-mcp)(CF₃SO₃)₂]: (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(22)	S(2)	O(4)	Mn(1)	-85.3(9)	O(4)	S(2)	C(22)	F(4)	57.1(8)
O(4)	S(2)	C(22)	F(5)	176.3(7)	O(4)	S(2)	C(22)	F(6)	-64.8(8)
O(5)	S(2)	C(22)	F(4)	-61.5(8)	O(5)	S(2)	C(22)	F(5)	57.7(8)
O(5)	S(2)	C(22)	F(6)	176.5(7)	O(6)	S(2)	C(22)	F(4)	176.1(7)
O(6)	S(2)	C(22)	F(5)	-64.8(8)	O(6)	S(2)	C(22)	F(6)	54.1(9)
Mn(1)	N(1)	C(2)	C(3)	41.4(6)	C(1)	N(1)	C(2)	C(3)	160.2(7)
C(8)	N(1)	C(2)	C(3)	-75.2(8)	Mn(1)	N(1)	C(8)	C(9)	169.4(5)
Mn(1)	N(1)	C(8)	C(18)	44.5(6)	C(1)	N(1)	C(8)	C(9)	46.6(9)
C(1)	N(1)	C(8)	C(18)	-78.3(8)	C(2)	N(1)	C(8)	C(9)	-75.2(8)
C(2)	N(1)	C(8)	C(18)	159.9(6)	Mn(1)	N(2)	C(3)	C(2)	-0.7(7)
Mn(1)	N(2)	C(3)	C(4)	174.4(5)	C(7)	N(2)	C(3)	C(2)	-175.6(7)
C(7)	N(2)	C(3)	C(4)	-0.5(1)	Mn(1)	N(2)	C(7)	C(6)	-172.9(5)
C(3)	N(2)	C(7)	C(6)	1.3(1)	Mn(1)	N(3)	C(12)	C(13)	39.6(6)
C(11)	N(3)	C(12)	C(13)	156.8(7)	C(18)	N(3)	C(12)	C(13)	-77.2(8)
Mn(1)	N(3)	C(18)	C(8)	37.8(6)	Mn(1)	N(3)	C(18)	C(19)	162.0(5)
C(11)	N(3)	C(18)	C(8)	-83.4(9)	C(11)	N(3)	C(18)	C(19)	40.8(1)
C(12)	N(3)	C(18)	C(8)	153.0(7)	C(12)	N(3)	C(18)	C(19)	-82.8(8)
Mn(1)	N(4)	C(13)	C(12)	7.7(7)	Mn(1)	N(4)	C(13)	C(14)	-173.9(5)
C(17)	N(4)	C(13)	C(12)	-175.5(7)	C(17)	N(4)	C(13)	C(14)	2.9(1)
Mn(1)	N(4)	C(17)	C(16)	175.5(5)	C(13)	N(4)	C(17)	C(16)	-1.0(1)
N(1)	C(2)	C(3)	N(2)	-29.0(9)	N(1)	C(2)	C(3)	C(4)	155.9(7)
N(2)	C(3)	C(4)	C(5)	-0.4(1)	C(2)	C(3)	C(4)	C(5)	174.4(7)
C(3)	C(4)	C(5)	C(6)	0.5(1)	C(4)	C(5)	C(6)	C(7)	0.3(1)
C(5)	C(6)	C(7)	N(2)	-1.2(1)	N(1)	C(8)	C(9)	C(10)	-179.0(6)
C(18)	C(8)	C(9)	C(10)	-55.0(9)	N(1)	C(8)	C(18)	N(3)	-56.8(8)
N(1)	C(8)	C(18)	C(19)	178.0(6)	C(9)	C(8)	C(18)	N(3)	177.2(6)
C(9)	C(8)	C(18)	C(19)	52.0(9)	C(8)	C(9)	C(10)	C(20)	59.0(1)
C(9)	C(10)	C(20)	C(19)	-60.2(1)	N(3)	C(12)	C(13)	N(4)	-33.5(9)
N(3)	C(12)	C(13)	C(14)	148.1(7)	N(4)	C(13)	C(14)	C(15)	-2.7(1)
C(12)	C(13)	C(14)	C(15)	175.6(7)	C(13)	C(14)	C(15)	C(16)	0.5(1)
C(14)	C(15)	C(16)	C(17)	1.3(1)	C(15)	C(16)	C(17)	N(4)	-1.1(1)
N(3)	C(18)	C(19)	C(20)	-179.2(7)	C(8)	C(18)	C(19)	C(20)	-54.8(1)
C(18)	C(19)	C(20)	C(10)	58.9(1)					

Crystallographic Data of $[\text{Mn}^{\text{II}}(\text{mep})(\text{CF}_3\text{SO}_3)_2]$:

Data Collection

A colorless rhombic crystal of $\text{MnS}_{2.6}\text{F}_6\text{O}_6\text{N}_4\text{C}_{18}\text{H}_{22}$ was mounted on a quartz fiber using Paratone N hydrocarbon oil. All measurements were made on a Bruker-Siemens SMART¹ CCD area detector with graphite monochromated Mo-K α radiation. Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the measured positions of 3401 reflections in the range $4^\circ < 2\theta < 43.94^\circ$, corresponded to a primitive orthorhombic cell with dimensions:

$$\begin{aligned}a &= 9.4259(6) \text{ \AA} \\b &= 17.4816(9) \text{ \AA} \\c &= 30.462(2) \text{ \AA} \\V &= 5019.6(4) \text{ \AA}^3\end{aligned}$$

For $Z = 8$ and F.W. = 623.44, the calculated density is 1.65 g/cm^3 . The systematic absences of:

$$\begin{aligned}0kl: k \pm 2n \\h0l: l \pm 2n \\hk0: h \pm 2n\end{aligned}$$

uniquely determine the space group to be:

$$\text{Pbca} (\#61)$$

The data were collected at a temperature of $-100 \pm 1^\circ \text{C}$ using the ω scan technique to a maximum 2θ value of 43.9° . Frames corresponding to an arbitrary hemisphere of data were collected using ω scans of 0.3° , counted for a total of 10 seconds per frame.

Data Reduction

Data were integrated by the program SAINT² with box parameters of 1.6×0.6 . Of the 22434 reflections which were collected, 3054 were unique ($R_{\text{int}} = 0.080$); equivalent reflections were merged. No decay correction was applied. The linear absorption coefficient, μ , for Mo-K α radiation is 7.8 cm^{-1} . Data were analyzed for agreement and possible absorption using SADABS³. A semi-empirical absorption correction based on 3382 reflections with $I > 10\sigma(I)$ was applied that resulted in transmission factors ranging from 0.78 to 0.97. The data were corrected for Lorentz and polarization effects.

Structure Solution and Refinement

The structure was solved by direct methods⁴ and expanded using Fourier techniques⁵. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were located by difference Fourier but were fixed at idealized positions $0.95 \text{ \AA}$ from their parent carbon atoms. The final cycle of full-matrix least-squares refinement⁶ on F^2 was based on 3054 observed reflections and 356 variable parameters and converged (largest parameter shift was less than 1% of its esd) with unweighted and weighted agreement factors of:

$$R_1 = \sum ||F_o| - |F_c|| / \sum |F_o| = 0.036$$

$$wR_2 = [\sum (w (F_o^2 - F_c^2)^2) / \sum w(F_o^2)^2]^{1/2} = 0.095$$

The standard deviation of an observation of unit weight⁷ was 0.69. The weighting scheme was based on counting statistics. Plots of $\sum w (|F_o| - |F_c|)^2$ versus $|F_o|$, reflection order in data collection, $\sin \theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.86 and $-0.65 \text{ e/\AA}^3$, respectively. The largest of these were located in the immediate vicinity of the thermally labile triflate ions. Neutral atom scattering factors were taken from Cromer and Waber⁸. Anomalous dispersion effects were included in F_c^9 ; the values for $\Delta f'$ and $\Delta f''$ were those of Creagh and McAuley¹⁰. The values for the mass attenuation coefficients are those of Creagh and Hubbell¹¹. All calculations were performed using the CrystalStructure^{12,13} crystallographic software package.

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	MnS ₂ F ₆ O ₆ N ₄ C ₁₈ H ₂₂
Formula Weight	623.44
Crystal Color, Habit	colorless rhombic
Crystal Dimensions	0.25 X 0.15 X 0.09 mm
Crystal System	orthorhombic
Lattice Type	Primitive
No. of Reflections Used for Unit	
Cell Determination (2 θ range)	3401 (4° < 2 θ < 43.94°)
Lattice Parameters	a = 9.4259(6) Å b = 17.4816(9) Å c = 30.462(2) Å V = 5019.6(4) Å ³
Space Group	Pbca (#61)
Z value	8
D _{calc}	1.650 g/cm ³
F ₀₀₀	2536.00
μ (MoK α)	7.79 cm ⁻¹

B. Intensity Measurements

Diffractometer	Bruker-Siemens SMART CCD
Radiation	MoK α (λ = 0.71069 Å) graphite monochromated
Temperature	-100° C
Scan Type	ω (0.3°/frame)
Scan Rate	10 sec Frame Exposure
2 θ _{max}	43.9°
No. of Reflections Measured	Total: 22434 Unique: 3054 (R _{int} = 0.080)
Corrections	Absorption, Lorentz, polarization

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELX97)
Refinement	Full-matrix least-squares on F ²
Function Minimized	$\sum w (F_o^2 - F_c^2)^2$
Least Squares Weights	$1/\sigma^2(F_o^2) = 1/\sigma^2(F_o)/(4F_o^2)$
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I > 0.00 σ (I))	3054
No. Variables	356
Reflection/Parameter Ratio	8.58
Residuals: R ₁ ; wR ₂	0.036 ; 0.095
Goodness of Fit Indicator	0.69
Max Shift/Error in Final Cycle	> 1%
Maximum peak in Final Diff. Map	0.86 e ⁻ /Å ³
Minimum peak in Final Diff. Map	-0.65 e ⁻ /Å ³

Table S21. Atomic coordinates and B_{iso}/B_{eq} for [Mn^{II}(**mep**)(CF₃SO₃)₂]:

atom	x	y	z	B _{eq}
Mn(1)	0.19592(7)	0.63365(4)	0.10951(2)	1.38(2)
S(1)	-0.0715(1)	0.52108(7)	0.15205(4)	1.66(3)
S(2)	-0.0585(1)	0.76624(7)	0.07467(4)	1.64(3)
F(1)	0.0162(4)	0.4875(2)	0.2311(1)	4.75(9)
F(2)	-0.2009(4)	0.4620(2)	0.2195(1)	5.8(1)
F(3)	-0.1352(4)	0.5777(2)	0.22901(9)	4.42(9)
F(4)	-0.0134(3)	0.8271(2)	0.15191(9)	3.61(8)
F(5)	-0.1419(4)	0.7270(2)	0.1535(1)	5.15(9)
F(6)	-0.2294(4)	0.8308(2)	0.1307(1)	6.5(1)
O(1)	0.0454(3)	0.5754(2)	0.1509(1)	2.20(8)
O(2)	-0.0341(4)	0.4454(2)	0.1384(1)	2.37(8)
O(3)	-0.2031(4)	0.5513(2)	0.1363(1)	3.45(9)
O(4)	0.0699(4)	0.7227(2)	0.0821(1)	3.9(1)
O(5)	-0.1736(4)	0.7238(2)	0.0565(1)	3.7(1)
O(6)	-0.0315(4)	0.8392(2)	0.0556(1)	3.35(9)
N(1)	0.1825(4)	0.5635(2)	0.0480(1)	1.63(9)
N(2)	0.3550(4)	0.5366(2)	0.1188(1)	1.57(9)
N(3)	0.4035(4)	0.6955(2)	0.0922(1)	1.75(9)
N(4)	0.2488(4)	0.7055(2)	0.1691(1)	1.58(9)
C(1)	0.1359(5)	0.5881(3)	0.0089(1)	2.1(1)
C(2)	0.1446(5)	0.5443(3)	-0.0291(1)	2.1(1)
C(3)	0.2020(5)	0.4723(3)	-0.0263(2)	2.4(1)
C(4)	0.2524(5)	0.4462(3)	0.0142(1)	2.1(1)
C(5)	0.2408(5)	0.4940(3)	0.0504(1)	1.5(1)
C(6)	0.2961(5)	0.4698(3)	0.0949(1)	1.8(1)
C(7)	0.3791(5)	0.5148(3)	0.1653(1)	2.4(1)
C(8)	0.4890(5)	0.5624(3)	0.0977(2)	2.2(1)
C(9)	0.5192(5)	0.6451(3)	0.1087(2)	2.2(1)
C(10)	0.4226(5)	0.7113(3)	0.0447(1)	2.8(1)
C(11)	0.4011(5)	0.7688(3)	0.1164(1)	2.4(1)
C(12)	0.3478(5)	0.7596(3)	0.1625(1)	1.9(1)
C(13)	0.3935(5)	0.8062(3)	0.1964(2)	2.6(1)
C(14)	0.3353(6)	0.7978(3)	0.2377(2)	3.0(1)
C(15)	0.2340(5)	0.7428(3)	0.2444(1)	2.5(1)
C(16)	0.1949(5)	0.6979(3)	0.2092(1)	2.0(1)
C(17)	-0.1005(6)	0.5116(3)	0.2111(2)	2.8(1)
C(18)	-0.1153(6)	0.7894(3)	0.1298(2)	2.7(1)

Table S21. Atomic coordinates and B_{iso}/B_{eq} for [Mn^{II}(**mep**)(CF₃SO₃)₂]: (continued)

atom	x	y	z	B _{eq}
H(1)	0.0943(5)	0.6375(3)	0.0074(1)	2.6(1)
H(2)	0.1124(5)	0.5639(3)	-0.0564(1)	2.5(1)
H(3)	0.2075(5)	0.4403(3)	-0.0515(2)	2.9(1)
H(4)	0.2924(5)	0.3966(3)	0.0170(1)	2.6(1)
H(5)	0.3684(5)	0.4324(3)	0.0913(1)	2.2(1)
H(6)	0.2204(5)	0.4486(3)	0.1115(1)	2.2(1)
H(7)	0.2920(5)	0.4998(3)	0.1784(1)	2.9(1)
H(8)	0.4444(5)	0.4735(3)	0.1664(1)	2.9(1)
H(9)	0.4171(5)	0.5573(3)	0.1808(1)	2.9(1)
H(10)	0.5652(5)	0.5315(3)	0.1079(2)	2.6(1)
H(11)	0.4803(5)	0.5570(3)	0.0668(2)	2.6(1)
H(12)	0.6056(5)	0.6604(3)	0.0952(2)	2.6(1)
H(13)	0.5269(5)	0.6505(3)	0.1396(2)	2.6(1)
H(14)	0.5101(5)	0.7374(3)	0.0407(1)	3.3(2)
H(15)	0.4238(5)	0.6649(3)	0.0285(1)	3.3(2)
H(16)	0.3470(5)	0.7427(3)	0.0346(1)	3.3(2)
H(17)	0.4948(5)	0.7889(3)	0.1174(1)	2.9(1)
H(18)	0.3412(5)	0.8035(3)	0.1011(1)	2.9(1)
H(19)	0.4649(5)	0.8434(3)	0.1911(2)	3.1(2)
H(20)	0.3660(6)	0.8293(3)	0.2614(2)	3.6(2)
H(21)	0.1924(5)	0.7362(3)	0.2725(1)	3.0(1)
H(22)	0.1252(5)	0.6595(3)	0.2137(1)	2.4(1)

$$B_{eq} = 8/3 \pi (U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa*bb*)\cos \gamma + 2U_{13}(aa*cc*)\cos \beta + 2U_{23}(bb*cc*)\cos \alpha)$$

Table S22. Anisotropic Displacement Parameters for [Mn^{II}(**mep**)(CF₃SO₃)₂]:

atom	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
Mn(1)	0.0164(4)	0.0202(4)	0.0160(4)	0.0005(3)	-0.0007(3)	-0.0017(4)
S(1)	0.0196(7)	0.0244(7)	0.0190(7)	-0.0042(6)	-0.0016(6)	0.0006(6)
S(2)	0.0204(7)	0.0221(7)	0.0198(7)	0.0014(6)	-0.0001(6)	0.0016(6)
F(1)	0.087(3)	0.071(2)	0.022(2)	0.025(2)	-0.014(2)	0.004(2)
F(2)	0.090(3)	0.069(3)	0.062(2)	-0.033(2)	0.047(2)	0.006(2)
F(3)	0.090(3)	0.043(2)	0.035(2)	0.017(2)	0.026(2)	-0.007(2)
F(4)	0.058(2)	0.048(2)	0.031(2)	-0.012(2)	-0.000(2)	-0.014(2)
F(5)	0.100(3)	0.055(2)	0.040(2)	-0.023(2)	0.031(2)	-0.001(2)
F(6)	0.061(3)	0.118(3)	0.070(2)	0.051(3)	0.003(2)	-0.035(2)
O(1)	0.027(2)	0.032(2)	0.025(2)	-0.014(2)	0.007(2)	-0.007(2)
O(2)	0.042(2)	0.018(2)	0.030(2)	-0.008(2)	0.003(2)	-0.007(2)
O(3)	0.025(2)	0.052(2)	0.054(3)	0.007(2)	-0.017(2)	0.006(2)
O(4)	0.052(3)	0.065(3)	0.032(2)	0.042(2)	-0.002(2)	-0.002(2)
O(5)	0.041(2)	0.063(3)	0.038(2)	-0.029(2)	-0.002(2)	-0.013(2)
O(6)	0.060(3)	0.034(2)	0.033(2)	-0.018(2)	-0.005(2)	0.008(2)
N(1)	0.018(2)	0.026(3)	0.017(2)	-0.004(2)	-0.002(2)	-0.000(2)
N(2)	0.020(2)	0.020(2)	0.019(2)	-0.001(2)	-0.003(2)	-0.003(2)
N(3)	0.026(2)	0.023(2)	0.018(2)	-0.003(2)	0.001(2)	-0.001(2)
N(4)	0.018(2)	0.024(2)	0.018(2)	0.002(2)	-0.001(2)	-0.006(2)
C(1)	0.025(3)	0.031(3)	0.024(3)	-0.002(2)	-0.003(2)	-0.001(3)
C(2)	0.025(3)	0.039(3)	0.016(3)	-0.003(3)	-0.005(2)	-0.003(3)
C(3)	0.018(3)	0.052(4)	0.023(3)	-0.005(3)	0.004(2)	-0.017(3)
C(4)	0.021(3)	0.029(3)	0.032(3)	0.000(2)	0.002(2)	-0.012(3)
C(5)	0.009(3)	0.024(3)	0.022(3)	-0.001(2)	0.003(2)	-0.001(2)
C(6)	0.023(3)	0.021(3)	0.026(3)	0.009(2)	0.002(2)	-0.001(2)
C(7)	0.039(3)	0.026(3)	0.026(3)	0.009(3)	-0.014(3)	0.000(2)
C(8)	0.016(3)	0.034(3)	0.033(3)	0.001(2)	-0.006(2)	-0.005(3)
C(9)	0.017(3)	0.038(3)	0.029(3)	-0.004(2)	0.002(2)	-0.006(3)
C(10)	0.041(3)	0.045(4)	0.019(3)	-0.010(3)	0.006(3)	0.001(3)
C(11)	0.041(3)	0.023(3)	0.027(3)	-0.007(3)	0.001(3)	0.001(2)
C(12)	0.028(3)	0.021(3)	0.025(3)	-0.003(3)	-0.005(2)	-0.003(2)
C(13)	0.039(3)	0.025(3)	0.035(3)	-0.009(3)	-0.008(3)	-0.003(3)
C(14)	0.054(4)	0.032(3)	0.028(4)	0.000(3)	-0.006(3)	-0.014(3)
C(15)	0.038(3)	0.040(3)	0.018(3)	0.002(3)	-0.002(2)	-0.001(3)
C(16)	0.026(3)	0.026(3)	0.023(3)	-0.003(3)	-0.002(3)	-0.001(2)
C(17)	0.046(4)	0.036(4)	0.025(3)	-0.001(3)	0.013(3)	0.002(3)
C(18)	0.037(4)	0.031(4)	0.035(3)	0.007(3)	0.004(3)	-0.009(3)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Table S23. Bond lengths (Å) for [Mn^{II}(**mep**)(CF₃SO₃)₂]:

atom	atom	distance	atom	atom	distance
Mn(1)	O(1)	2.154(3)	Mn(1)	O(4)	2.128(3)
Mn(1)	N(1)	2.243(4)	Mn(1)	N(2)	2.282(4)
Mn(1)	N(3)	2.296(4)	Mn(1)	N(4)	2.262(3)
S(1)	O(1)	1.455(3)	S(1)	O(2)	1.431(3)
S(1)	O(3)	1.431(3)	S(1)	C(17)	1.827(5)
S(2)	O(4)	1.448(3)	S(2)	O(5)	1.425(3)
S(2)	O(6)	1.424(3)	S(2)	C(18)	1.810(5)
F(1)	C(17)	1.327(6)	F(2)	C(17)	1.308(6)
F(3)	C(17)	1.319(6)	F(4)	C(18)	1.345(6)
F(5)	C(18)	1.331(6)	F(6)	C(18)	1.296(6)
N(1)	C(1)	1.341(6)	N(1)	C(5)	1.335(6)
N(2)	C(6)	1.484(5)	N(2)	C(7)	1.485(6)
N(2)	C(8)	1.488(5)	N(3)	C(9)	1.488(6)
N(3)	C(10)	1.485(5)	N(3)	C(11)	1.479(5)
N(4)	C(12)	1.344(5)	N(4)	C(16)	1.331(6)
C(1)	C(2)	1.388(6)	C(2)	C(3)	1.374(6)
C(3)	C(4)	1.398(7)	C(4)	C(5)	1.390(6)
C(5)	C(6)	1.513(6)	C(8)	C(9)	1.512(6)
C(11)	C(12)	1.502(6)	C(12)	C(13)	1.384(6)
C(13)	C(14)	1.380(7)	C(14)	C(15)	1.371(7)
C(15)	C(16)	1.378(6)			

Table S24. Bond lengths involving hydrogens (Å) for [Mn^{II}(**mep**)(CF₃SO₃)₂]:

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.950(6)	C(2)	H(2)	0.950(6)
C(3)	H(3)	0.950(7)	C(4)	H(4)	0.950(6)
C(6)	H(5)	0.950(6)	C(6)	H(6)	0.950(6)
C(7)	H(7)	0.950(6)	C(7)	H(8)	0.950(6)
C(7)	H(9)	0.950(6)	C(8)	H(10)	0.950(6)
C(8)	H(11)	0.95	C(9)	H(12)	0.95
C(9)	H(13)	0.95	C(10)	H(14)	0.95
C(10)	H(15)	0.95	C(10)	H(16)	0.95
C(11)	H(17)	0.95	C(11)	H(18)	0.95
C(13)	H(19)	0.950(7)	C(14)	H(20)	0.950(7)
C(15)	H(21)	0.950(6)	C(16)	H(22)	0.950(6)

Table S25. Bond angles (°) for [Mn^{II}(**mep**)(CF₃SO₃)₂]:

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Mn(1)	O(4)	102.0(1)	O(1)	Mn(1)	N(1)	101.2(1)
O(4)	Mn(1)	N(1)	92.3(1)	O(1)	Mn(1)	N(2)	90.5(1)
O(4)	Mn(1)	N(2)	163.5(1)	N(1)	Mn(1)	N(2)	74.6(1)
O(1)	Mn(1)	N(3)	156.6(1)	O(4)	Mn(1)	N(3)	92.4(1)
N(1)	Mn(1)	N(3)	96.5(1)	N(2)	Mn(1)	N(3)	79.5(1)
O(1)	Mn(1)	N(4)	86.4(1)	O(4)	Mn(1)	N(4)	91.8(1)
N(1)	Mn(1)	N(4)	170.4(1)	N(2)	Mn(1)	N(4)	99.7(1)
N(3)	Mn(1)	N(4)	74.6(1)	O(1)	S(1)	O(2)	114.2(2)
O(1)	S(1)	O(3)	114.0(2)	O(2)	S(1)	O(3)	117.2(2)
O(1)	S(1)	C(17)	101.3(2)	O(2)	S(1)	C(17)	103.8(2)
O(3)	S(1)	C(17)	103.5(2)	O(4)	S(2)	O(5)	115.0(2)
O(4)	S(2)	O(6)	112.6(2)	O(5)	S(2)	O(6)	116.3(2)
O(4)	S(2)	C(18)	102.7(2)	O(5)	S(2)	C(18)	104.6(2)
O(6)	S(2)	C(18)	103.4(2)	Mn(1)	O(1)	S(1)	145.2(2)
Mn(1)	O(4)	S(2)	155.8(3)	Mn(1)	N(1)	C(1)	125.9(3)
Mn(1)	N(1)	C(5)	115.3(3)	C(1)	N(1)	C(5)	118.4(4)
Mn(1)	N(2)	C(6)	106.2(3)	Mn(1)	N(2)	C(7)	114.2(3)
C(6)	N(2)	C(7)	108.9(3)	Mn(1)	N(2)	C(8)	106.2(3)
C(6)	N(2)	C(8)	110.2(4)	C(7)	N(2)	C(8)	111.1(4)
Mn(1)	N(3)	C(9)	105.6(3)	Mn(1)	N(3)	C(10)	114.5(3)
C(9)	N(3)	C(10)	110.5(4)	Mn(1)	N(3)	C(11)	106.3(3)
C(9)	N(3)	C(11)	110.9(4)	C(10)	N(3)	C(11)	108.9(4)
Mn(1)	N(4)	C(12)	115.2(3)	Mn(1)	N(4)	C(16)	126.7(3)
C(12)	N(4)	C(16)	118.1(4)	N(1)	C(1)	C(2)	123.0(5)
C(1)	C(2)	C(3)	118.6(5)	C(2)	C(3)	C(4)	119.1(4)
C(3)	C(4)	C(5)	118.6(5)	N(1)	C(5)	C(4)	122.4(4)
N(1)	C(5)	C(6)	116.5(4)	C(4)	C(5)	C(6)	121.1(4)
N(2)	C(6)	C(5)	110.3(4)	N(2)	C(8)	C(9)	110.7(4)
N(3)	C(9)	C(8)	110.7(4)	N(3)	C(11)	C(12)	112.2(4)
N(4)	C(12)	C(11)	116.5(4)	N(4)	C(12)	C(13)	121.3(4)
C(11)	C(12)	C(13)	122.1(4)	C(12)	C(13)	C(14)	119.6(5)
C(13)	C(14)	C(15)	119.0(5)	C(14)	C(15)	C(16)	118.2(5)
N(4)	C(16)	C(15)	123.8(5)	S(1)	C(17)	F(1)	110.9(4)
S(1)	C(17)	F(2)	111.1(4)	F(1)	C(17)	F(2)	107.4(4)
S(1)	C(17)	F(3)	111.4(4)	F(1)	C(17)	F(3)	107.1(5)
F(2)	C(17)	F(3)	108.7(4)	S(2)	C(18)	F(4)	111.3(4)
S(2)	C(18)	F(5)	112.0(4)	F(4)	C(18)	F(5)	105.4(4)
S(2)	C(18)	F(6)	112.9(4)	F(4)	C(18)	F(6)	108.0(4)
F(5)	C(18)	F(6)	106.9(5)				

Table S26. Bond angles involving hydrogens (°) for [Mn^{II}(**mep**)(CF₃SO₃)₂]:

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(1)	H(1)	119.1(3)	C(1)	C(2)	H(2)	120.8(3)
C(3)	C(2)	H(2)	120.6(3)	C(2)	C(3)	H(3)	120.8(3)
C(4)	C(3)	H(3)	120.1(3)	C(3)	C(4)	H(4)	120.8(3)
C(5)	C(4)	H(4)	120.5(3)	N(2)	C(6)	H(5)	109.2(2)
C(5)	C(6)	H(5)	109.6(2)	N(2)	C(6)	H(6)	109.1(2)
C(5)	C(6)	H(6)	109.1(2)	H(5)	C(6)	H(6)	109.5
N(2)	C(7)	H(7)	109.8(2)	N(2)	C(7)	H(8)	109.2(2)
H(7)	C(7)	H(8)	109.5(2)	N(2)	C(7)	H(9)	109.4(2)
H(7)	C(7)	H(9)	109.5(2)	H(8)	C(7)	H(9)	109.5
N(2)	C(8)	H(10)	109.1(2)	C(9)	C(8)	H(10)	109.2(3)
N(2)	C(8)	H(11)	109.0(2)	C(9)	C(8)	H(11)	109.3(3)
H(10)	C(8)	H(11)	109.5	N(3)	C(9)	H(12)	108.5(2)
C(8)	C(9)	H(12)	109.6(3)	N(3)	C(9)	H(13)	109.3(2)
C(8)	C(9)	H(13)	109.3(3)	H(12)	C(9)	H(13)	109.5
N(3)	C(10)	H(14)	108.6(2)	N(3)	C(10)	H(15)	110.4(3)
H(14)	C(10)	H(15)	109.5	N(3)	C(10)	H(16)	109.4(3)
H(14)	C(10)	H(16)	109.5	H(15)	C(10)	H(16)	109.5
N(3)	C(11)	H(17)	108.8(3)	C(12)	C(11)	H(17)	108.7(3)
N(3)	C(11)	H(18)	108.7(2)	C(12)	C(11)	H(18)	109.1(3)
H(17)	C(11)	H(18)	109.5(3)	C(12)	C(13)	H(19)	119.6(3)
C(14)	C(13)	H(19)	120.8(3)	C(13)	C(14)	H(20)	120.5(3)
C(15)	C(14)	H(20)	120.4(3)	C(14)	C(15)	H(21)	120.4(3)
C(16)	C(15)	H(21)	121.4(3)	N(4)	C(16)	H(22)	117.8(3)
C(15)	C(16)	H(22)	118.4(3)				

Table S27. Torsion Angles (°) for [Mn^{II}(**mep**)(CF₃SO₃)₂]:

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(4)	Mn(1)	O(1)	S(1)	79.0(8)	N(1)	Mn(1)	O(1)	S(1)	-15.8(9)
N(2)	Mn(1)	O(1)	S(1)	-90.2(8)	N(3)	Mn(1)	O(1)	S(1)	-154.3(8)
N(4)	Mn(1)	O(1)	S(1)	170.1(7)	O(1)	Mn(1)	O(4)	S(2)	-1.6(1)
N(1)	Mn(1)	O(4)	S(2)	100.3(1)	N(2)	Mn(1)	O(4)	S(2)	137.0(1)
N(3)	Mn(1)	O(4)	S(2)	-163.0(1)	N(4)	Mn(1)	O(4)	S(2)	-88.3(1)
O(1)	Mn(1)	N(1)	C(1)	115.5(7)	O(1)	Mn(1)	N(1)	C(5)	-72.0(6)
O(4)	Mn(1)	N(1)	C(1)	12.8(8)	O(4)	Mn(1)	N(1)	C(5)	-174.7(6)
N(2)	Mn(1)	N(1)	C(1)	-157.1(7)	N(2)	Mn(1)	N(1)	C(5)	15.4(6)
N(3)	Mn(1)	N(1)	C(1)	-79.8(7)	N(3)	Mn(1)	N(1)	C(5)	92.6(6)
N(4)	Mn(1)	N(1)	C(1)	-102.6(3)	N(4)	Mn(1)	N(1)	C(5)	69.9(3)
O(1)	Mn(1)	N(2)	C(6)	69.7(5)	O(1)	Mn(1)	N(2)	C(7)	-50.3(6)
O(1)	Mn(1)	N(2)	C(8)	-173.1(5)	O(4)	Mn(1)	N(2)	C(6)	-70.0(2)
O(4)	Mn(1)	N(2)	C(7)	170.0(1)	O(4)	Mn(1)	N(2)	C(8)	47.2(2)
N(1)	Mn(1)	N(2)	C(6)	-31.8(5)	N(1)	Mn(1)	N(2)	C(7)	-151.8(6)
N(1)	Mn(1)	N(2)	C(8)	85.4(5)	N(3)	Mn(1)	N(2)	C(6)	-131.7(5)
N(3)	Mn(1)	N(2)	C(7)	108.4(6)	N(3)	Mn(1)	N(2)	C(8)	-14.4(5)
N(4)	Mn(1)	N(2)	C(6)	156.1(5)	N(4)	Mn(1)	N(2)	C(7)	36.2(6)
N(4)	Mn(1)	N(2)	C(8)	-86.6(6)	O(1)	Mn(1)	N(3)	C(9)	51.0(1)
O(1)	Mn(1)	N(3)	C(10)	172.8(9)	O(1)	Mn(1)	N(3)	C(11)	-66.9(1)
O(4)	Mn(1)	N(3)	C(9)	179.3(5)	O(4)	Mn(1)	N(3)	C(10)	-59.0(6)
O(4)	Mn(1)	N(3)	C(11)	61.4(6)	N(1)	Mn(1)	N(3)	C(9)	-88.1(6)
N(1)	Mn(1)	N(3)	C(10)	33.6(7)	N(1)	Mn(1)	N(3)	C(11)	154.0(5)
N(2)	Mn(1)	N(3)	C(9)	-15.2(5)	N(2)	Mn(1)	N(3)	C(10)	106.6(6)
N(2)	Mn(1)	N(3)	C(11)	-133.1(6)	N(4)	Mn(1)	N(3)	C(9)	88.0(5)
N(4)	Mn(1)	N(3)	C(10)	-150.2(6)	N(4)	Mn(1)	N(3)	C(11)	-29.9(5)
O(1)	Mn(1)	N(4)	C(12)	-179.2(6)	O(1)	Mn(1)	N(4)	C(16)	2.6(7)
O(4)	Mn(1)	N(4)	C(12)	-77.3(6)	O(4)	Mn(1)	N(4)	C(16)	104.5(7)
N(1)	Mn(1)	N(4)	C(12)	38.2(3)	N(1)	Mn(1)	N(4)	C(16)	-140.0(3)
N(2)	Mn(1)	N(4)	C(12)	90.9(6)	N(2)	Mn(1)	N(4)	C(16)	-87.3(7)
N(3)	Mn(1)	N(4)	C(12)	14.7(6)	N(3)	Mn(1)	N(4)	C(16)	-163.5(7)
O(2)	S(1)	O(1)	Mn(1)	63.5(7)	O(3)	S(1)	O(1)	Mn(1)	-75.1(7)
C(17)	S(1)	O(1)	Mn(1)	174.4(5)	O(1)	S(1)	C(17)	F(1)	-58.5(7)
O(1)	S(1)	C(17)	F(2)	-177.8(6)	O(1)	S(1)	C(17)	F(3)	60.8(7)
O(2)	S(1)	C(17)	F(1)	60.3(7)	O(2)	S(1)	C(17)	F(2)	-59.1(8)
O(2)	S(1)	C(17)	F(3)	179.5(6)	O(3)	S(1)	C(17)	F(1)	-176.8(6)
O(3)	S(1)	C(17)	F(2)	63.8(8)	O(3)	S(1)	C(17)	F(3)	-57.6(8)
O(5)	S(2)	O(4)	Mn(1)	-59.4(1)	O(6)	S(2)	O(4)	Mn(1)	164.2(8)

Table S27. Torsion angles (°) for [Mn^{II}(**mep**)(CF₃SO₃)₂]: (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(18)	S(2)	O(4)	Mn(1)	53.6(1)	O(4)	S(2)	C(18)	F(4)	56.8(8)
O(4)	S(2)	C(18)	F(5)	-60.8(8)	O(4)	S(2)	C(18)	F(6)	178.4(6)
O(5)	S(2)	C(18)	F(4)	177.3(6)	O(5)	S(2)	C(18)	F(5)	59.6(8)
O(5)	S(2)	C(18)	F(6)	-61.1(8)	O(6)	S(2)	C(18)	F(4)	-60.5(7)
O(6)	S(2)	C(18)	F(5)	-178.2(6)	O(6)	S(2)	C(18)	F(6)	61.1(8)
Mn(1)	N(1)	C(1)	C(2)	172.8(4)	C(5)	N(1)	C(1)	C(2)	0.5(9)
Mn(1)	N(1)	C(5)	C(4)	-174.2(4)	Mn(1)	N(1)	C(5)	C(6)	5.0(6)
C(1)	N(1)	C(5)	C(4)	-1.2(9)	C(1)	N(1)	C(5)	C(6)	178.1(5)
Mn(1)	N(2)	C(6)	C(5)	44.5(5)	C(7)	N(2)	C(6)	C(5)	167.8(5)
C(8)	N(2)	C(6)	C(5)	-70.1(7)	Mn(1)	N(2)	C(8)	C(9)	42.8(5)
C(6)	N(2)	C(8)	C(9)	157.3(5)	C(7)	N(2)	C(8)	C(9)	-81.9(7)
Mn(1)	N(3)	C(9)	C(8)	43.4(5)	C(10)	N(3)	C(9)	C(8)	-80.9(7)
C(11)	N(3)	C(9)	C(8)	158.2(6)	Mn(1)	N(3)	C(11)	C(12)	42.4(5)
C(9)	N(3)	C(11)	C(12)	-72.0(7)	C(10)	N(3)	C(11)	C(12)	166.3(6)
Mn(1)	N(4)	C(12)	C(11)	4.5(6)	Mn(1)	N(4)	C(12)	C(13)	-178.1(4)
C(16)	N(4)	C(12)	C(11)	-177.2(6)	C(16)	N(4)	C(12)	C(13)	0.3(9)
Mn(1)	N(4)	C(16)	C(15)	178.6(4)	C(12)	N(4)	C(16)	C(15)	0.5(1)
N(1)	C(1)	C(2)	C(3)	0.8(9)	C(1)	C(2)	C(3)	C(4)	-1.4(9)
C(2)	C(3)	C(4)	C(5)	0.8(9)	C(3)	C(4)	C(5)	N(1)	0.5(1)
C(3)	C(4)	C(5)	C(6)	-178.8(6)	N(1)	C(5)	C(6)	N(2)	-34.7(7)
C(4)	C(5)	C(6)	N(2)	144.6(6)	N(2)	C(8)	C(9)	N(3)	-61.1(6)
N(3)	C(11)	C(12)	N(4)	-33.0(7)	N(3)	C(11)	C(12)	C(13)	149.6(6)
N(4)	C(12)	C(13)	C(14)	-0.8(9)	C(11)	C(12)	C(13)	C(14)	176.5(6)
C(12)	C(13)	C(14)	C(15)	0.5(1)	C(13)	C(14)	C(15)	C(16)	0.2(1)
C(14)	C(15)	C(16)	N(4)	-0.7(1)					

Crystallographic References

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- (6) Least Squares function minimized:
$$\sum w(F_o^2 - F_c^2)^2 \quad \text{where } w = \text{Least Squares weights.}$$
- (7) Standard deviation of an observation of unit weight:
$$[\sum w(F_o^2 - F_c^2)^2 / (N_O - N_V)]^{1/2}$$
where: N_O = number of observations
 N_V = number of variables
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- (13) CRYSTALS Issue 10: Watkin, D.J., Prout, C.K. Carruthers, J.R. & Betteridge, P.W. Chemical Crystallography Laboratory, Oxford, UK.

Experimental

All olefins were purchased from Aldrich and distilled prior to use. 32% peracetic acid (Aldrich) was used directly. Gas chromatographic (GC) yields were determined using either a DB-5 capillary column [30m x 0.53 mm x 5 μ m, He 15 psi] or DB-1 capillary column [15m x 0.25 mm x 0.1 μ m, He 10 psi] on a HP 5890 GC. GC conditions for each substrate are listed below. Large-scale reactions were performed in high surface to volume flasks (e.g. Erlenmeyer flasks) with external cooling to assure appropriate heat dissipation. Isolated products were > 97% pure by GC.

Epoxidation of Alkenes with **1** on GC Scale

An MeCN (0.1 mL) solution of alkene (0.05 mmole, 0.5 M), **1** (5×10^{-8} moles, 5 mM), and *tert*-butylbenzene (internal standard, 5 mol%, 0.0025 mmole, 0.025 M) was prepared in a 0.3 mL conical vial at RT with a stirbar. 1.2 equivalents of 32% peracetic acid (14.2 mg, 0.06 mmole, 13.2 μ L) was added dropwise over 30 seconds. The reaction was stirred for 5 minutes, diluted with Et₂O, and filtered through a basic alumina plug. The GC analysis of the solution provides the substrate conversion and product yield relative to the internal standard integration. The epoxide product was identified by a comparison of the GC retention time of an authentic sample and the reaction sample. In cases in which authentic samples were not readily available, the structures were assigned through a combination of GC/MS and ¹H NMR of an isolated sample.

GC Conditions:

Cyclooctene: 150° C isothermal for 10 minutes on DB-5 column. Cyclooctene R_t = 1.84 minutes, cyclooctene oxide R_t = 3.24 minutes. Product identity was confirmed with comparison to an authentic samples (Aldrich, 99% cyclooctene R_t = 3.24 minutes) and GC/MS ([m/z] = 126)

Cyclohexene: 120° C isothermal for 10 minutes on DB-5 column. Cyclohexene R_t = 1.23 minutes, cyclohexene oxide R_t = 2.25 minutes. Product identity was confirmed with comparison to an authentic samples (Aldrich, 98% cyclohexene oxide, R_t = 2.25 minutes) and GC/MS ([m/z] = 98).

Vinyl Cyclohexane: 150° C isothermal for 10 minutes on DB-5 column. Vinyl cyclohexane R_t = 1.46 minutes, 1,2-epoxyethylcyclohexane R_t = 2.79 minutes. Product identity confirmed by GC/MS ([m/z] = 126) and by ¹H NMR.⁶

1-Methyl-1-cyclohexene: 150° C isothermal for 10 minutes on DB-5 column. 1-Methyl-1-cyclohexene R_t = 1.5 minutes. 1-Methyl-1-cyclohexene oxide R_t = 2.33 minutes. Product identity confirmed by GC/MS ([m/z] = 112) and ¹H NMR.⁷

cis-2-heptene: 120° C isothermal for 10 minutes on DB-5 column. *Cis*-2-heptene R_t = 1.3 minutes, *cis*-2,3-epoxy heptane R_t = 2.33, *trans*-2,3 heptane R_t = 2.08 minutes. Product identity confirmed by GC/MS ([m/z] = 114) and by ¹H NMR.⁶

trans-2-heptene: 120° C isothermal for 10 minutes on DB-5 column. *Trans*-2-heptene R_t = 1.27 minutes, *trans*-2,3-epoxyheptane R_t = 2.08 minutes, *cis*-2,3-epoxyheptane R_t = 2.33 minutes. Product identity confirmed GC/MS ([m/z] = 114) and by ¹H NMR.⁷

Allyl acetate: 100° C isothermal for 10 minutes on DB-5 column. Allyl acetate R_t = 1.51 minutes, 1,2-epoxypropyl acetate R_t = 3.75 minutes. Product identity confirmed GC/MS ([m/z] = 116) and by ¹H NMR.⁸

2-Methyl-1-pentene: 60° C (5 minutes), 25° C/Min, 150° C (5 minutes) on DB-5 column. 2-methyl-1-pentene R_t = 1.94 minutes, 1,2-epoxy-2-methyl-pentane R_t = 4.89 minutes. Product identity confirmed GC/MS ([m/z] = 100) and by ¹H NMR.⁷

1-Heptene: 120° C isothermal for 10 minutes on DB-5 column. 1-heptene R_t = 1.22 minutes, 1,2-epoxyheptane R_t = 2.68 minutes. Product identity confirmed GC/MS ([m/z] = 114) and by ¹H NMR.⁶

2-Cyclohexen-1-one: 130° C isothermal for 10 minutes on DB-5 column. 2-cyclohexene-1-one R_t = 1.84 minutes, 2,3-epoxy-cyclohexanone R_t = 3.26 minutes. Product identity confirmed by GC/MS ([m/z] = 112) and ¹H NMR.⁹

Methyl methacrylate: 120° C isothermal for 10 minutes on DB-5 Column. Methyl methacrylate R_t = 1.22, methyl 2-methylglycidate R_t = 1.83. Product identity confirmed by GC/MS ([m/z] = 116) and ¹H NMR.¹⁰

Trans- β -methylstyrene: 70° C isothermal for 10 minutes on DB-1 column. *Trans*- β -methylstyrene R_t = 1.73 min, *trans*- β -methylstyrene oxide R_t = 3.11 min, *cis*- β -methylstyrene R_t = 2.82 min. Product confirmed by GC/MS ([m/z] = 134) and by ¹H NMR.

Cis- β -methylstyrene: 70°C isothermal for 10 minutes on DB-1 column. *Cis*- β -methylstyrene R_t = 1.41 min, *cis*- β -methylstyrene R_t = 2.82 min, *trans*- β -methylstyrene oxide R_t = 3.11 min. Product confirmed by GC/MS ($[m/z]$ = 134) and by ^1H NMR.

Ethyl Sorbate: 80°C isothermal for 10 minutes on DB-1 column. Ethyl Sorbate R_t = 1.07 min, 4,5-epoxy-ethyl sorbate R_t = 3.27 min, 2,3-epoxy-ethyl sorbate R_t = 3.37 min. Product confirmed by GC/MS ($[m/z]$ = 156) and by ^1H NMR.

***R*-(-)-Carvone (diepoxide product):** 120°C isothermal for 10 minutes on DB-1 column. *R*-(-)-Carvone R_t = 1.21 min, 2-Methyl-5-(2-methyl-oxiranyl)-cyclohex-2-enone R_t = 2.46, 2.49 (diastereomers), 1-Methyl-4-(2-methyl-oxiranyl)-7-oxa-bicyclo[4.1.0]heptan-2-one (carvone diepoxide) R_t = 2.84, 2.99 (diastereomers). Product confirmed GC/MS ($[m/z]$ = 184) and by ^1H NMR.¹¹⁻¹⁴

***R*-(-)-Carvone (monoepoxide product):** 80°C isothermal for 25 minutes on DB-1 column. *R*-(-)-Carvone R_t = 6.95 min, 2-Methyl-5-(2-methyl-oxiranyl)-cyclohex-2-enone R_t = 13.315, 13.653 (diastereomers). Product confirmed GC/MS ($[m/z]$ = 168) and by ^1H NMR.¹¹⁻¹⁴

Gram-scale Epoxidations:

Methyl Methacrylate

Caution this reaction is very exothermic

A mixture of methyl methacrylate (1.0 g, 0.01 mole), ***R,R*-mcp** (6.4 mg, 0.02 mmole), $\text{Mn}(\text{OAc})_2 \cdot 4 \text{H}_2\text{O}$ (4.9 mg, 0.02 mmole), and 20 mL of MeCN was stirred in a 125 mL Erlenmeyer flask at RT until homogeneous. The solution was cooled in an ice bath, and 32% peracetic acid (3.57g, 0.015 moles) was added dropwise with stirring over 2 minutes. After an additional 3 minutes, the reaction flask was removed from the ice bath and allowed to warm to RT. The solution was carefully diluted with saturated NaHCO_3 (40 mL) and extracted with Et_2O (2 x 50 mL). The combined organic volume was washed with H_2O (2 x 50 mL) and dried over Na_2SO_4 . Removal of the organic solvent under vacuum gave 0.99 g of the desired epoxide product (86%). $[m/z]$ = 116. ^1H NMR (CD_3Cl): δ = 3.71 (3H, s), 3.1 (1H, d), 2.76 (1H, d), 1.99 (3H, s). ^{13}C NMR (CD_3Cl) δ = 171.2, 53.7, 53.02, 52.64, 17.43.

Vinyl Cyclohexane

Caution this reaction is very exothermic

A mixture containing $\text{Mn}(\text{CF}_3\text{SO}_3)_2$ (0.0032 g, 9.1×10^{-6} mole), ***R,R*-mcp** (0.003 g, 9.1×10^{-6} mole), vinyl cyclohexane (1 g, 0.0093 mole), and 9 mL of MeCN was stirred in a 125 mL Erlenmeyer flask at RT until homogeneous. The solution was cooled in an ice bath, and 32% peracetic acid (2.59 g, 0.011 mole, 1.2 equivalents) was added via a syringe over the course of 3 minutes with stirring. After an additional 3 minutes, the reaction flask was removed from the ice bath and allowed to warm to RT. The solution was carefully diluted with saturated NaHCO_3 (10 mL) and extracted with pentane (2 x 40 mL). The combined organic volume was washed with saturated NaHCO_3 (2 x 50 mL), dried over K_2CO_3 , and filtered through a glass frit. Removal of the solvent under vacuum gave 1.05 g of 1,2 epoxy ethylcyclohexane (90%, 1.14 g theoretical). $[m/z]$ = 126. ^1H NMR (CD_3Cl) δ = 2.71 (2H, m), 2.52 (1H, t), 1.88 (1H, dd), 1.75-1.65 (4H, m), 1.28-1.1 (6H, m), 0.9 (1H, t). ^{13}C NMR CD_3Cl : δ = 56.7, 46.0, 40.4, 29.7, 28.9, 26.3, 25.7, 25.5.

2-Cyclohexen-1-one

Caution this reaction is very exothermic

A mixture containing $\text{Mn}(\text{CF}_3\text{SO}_3)_2$ (0.0185 g, 0.0005 mole), ***R,R*-mcp** (0.017 g, 0.0005 mole), 2-cyclohexen-1-one (1 g, 0.0104 mole), and 10 mL of MeCN was stirred in a 125 mL Erlenmeyer flask at RT until homogeneous. The solution was cooled in an ice bath, and 32% peracetic acid (4.95g, 0.020 mole, 2 equivalents) was added via a syringe over the course of 3

minutes with stirring. After an additional 10 minutes, the reaction flask was removed from the ice bath and allowed to warm to RT. The solution was carefully diluted with saturated NaHCO₃ (10 mL) and extracted with Et₂O (3 x 30 mL). The combined organic volume was washed with saturated NaHCO₃ (2 x 50 mL) and dried over MgSO₄. Removal of the solvent under vacuum gave 1.01 g of 2,3-epoxy-cyclohexa-1-one (88%, 1.15 g theoretical). [m/z] = 126. ¹H NMR (CD₃Cl) δ = 4.12 (1H, d), 3.66 (1H, dd), 2.2-3.0 (6H, m). ¹³C NMR (CD₃Cl) δ = 206.1, 56.2, 55.38, 36.71, 23.01, 17.03.

***R*-(-)-carvone to *R*-(-)-carvone-diepoxide**

Caution this reaction is very exothermic

A mixture containing Mn(CF₃SO₃)₂ (0.012 g, 0.00037 mole), ***R,R*-mcp** (0.011 g, 0.00037 mole), *R*-(-)-carvone (1 g, 0.067 mole), and 20 mL of MeCN was stirred in a 125 mL Erlenmeyer flask at RT until homogeneous. The solution was cooled in an ice bath, and 32% peracetic acid (4.75g, 0.019 mole, 3 equivalents) was added via a syringe over the course of 3 minutes to insure the temperature did not rise above 10°C. After an additional 10 minutes, the reaction flask was removed from the ice bath and allowed to warm to RT. The reaction was quenched by the addition of 3 g potassium carbonate in 100 mL of H₂O and extracted with Et₂O (3 x 75 mL). The combined organic volume was washed with saturated NaHCO₃ (2 x 50 mL) and dried over MgSO₄. Removal of the organic solvent under vacuum gave 1.06 g of carvone-diepoxide (88%, 1.21 g theoretical). The diastereoselectivity of the terminal olefin oxidation was determined by integration of the ¹H NMR features at 2.66 and 2.62 ppm, *de* = 17%. A slightly higher *de* (20%) was obtained by comparing the 2.84 and 2.99 min GC peaks. [m/z] = 182. ¹H NMR (CD₃Cl) δ = 3.43 (1H, d), 2.7-1.8 (7H, m), 1.40 (3H, s), 1.27 (3H, d). ¹³C NMR (CD₃Cl) δ = 204.76, 60.95, 60.84, 58.98, 58.93, 57.70, 57.60, 52.88, 52.22, 38.78, 38.29, 33.56, 25.35, 25.24, 18.81, 18.55, 15.15.

***R*-(-)-carvone to *R*-(-)-carvone 8,9-monoepoxide**

Caution this reaction is very exothermic

A mixture containing Mn(CF₃SO₃)₂ (0.012 g, 0.00037 mole), ***R,R*-mcp** (0.011 g, 0.00037 mole), *R*-(-)-carvone (1 g, 0.067 mole), and 14 mL of MeCN was stirred in a 125 mL Erlenmeyer flask at RT until homogeneous. The solution was cooled to -20°C in a cooling bath, and 32% peracetic acid solution (1.67 g, 0.0067 mole, 1 equivalent) was added via a syringe over the course of 3 minutes to insure the temperature did not rise above -10°C. After an additional 10 minutes, the cooling bath was removed, and the reaction flask was allowed to warm to RT. The reaction was quenched by the careful addition of 3 g K₂CO₃ in 100 mL H₂O and extracted with Et₂O (3 x 75 mL). The combined organic volume was washed with saturated NaHCO₃ (2 x 50 mL) and dried over MgSO₄. Removal of the organic solvent under vacuum gave 1.05 g of carvone-8,9-oxide (93%, 1.12 g theoretical). The diastereoselectivity (*de*) of the terminal olefin oxidation was determined by the integrations of the ¹H NMR features at 2.66 and 2.62 ppm, *de* = 15%. A *de* (15%) was obtained by comparing the 13.32 and 13.65 min GC peaks. [m/z] = 166. ¹H NMR (CD₃Cl) δ = 6.6 (1H, s), 2.6-1.8 (7H, m), 1.65 (3H, s), 1.20 (3H, d). ¹³C NMR (CD₃Cl) δ = 198.53, 144.00, 143.77, 135.24, 135.20, 57.69, 57.59, 52.56, 52.19, 40.99, 40.52, 39.63, 38.65, 27.66, 27.46, 18.62, 18.25, 15.42.

Cyclohexene

Caution this reaction is very exothermic

A solution containing Mn(CF₃SO₃)₂ (0.0037 g, 1.2 x 10⁻⁵ mole), ***R,R*-mcp** (0.003.3 g, 1.2 x 10⁻⁵ mole), cyclohexene (1.0 g 0.0121 mole), and 12 mL of MeCN was stirred in a 125 mL Erlenmeyer flask at RT until homogeneous. The solution was cooled in an ice bath, and 32% peracetic acid (2.67g, 0.011 mole, 1.2 equivalents) was added via a syringe over the course of 3 minutes. After an additional 3 minutes, the reaction flask was removed from the ice bath and allowed to warm to RT. The solution was carefully diluted with saturated NaHCO₃ (5 mL) and extracted with pentane (3 x 50 mL). The combined organic volume was washed with saturated NaHCO₃ (2 x 50 mL), dried over K₂CO₃, and filtered through a glass frit. Removal of the solvent under vacuum gave 1.01 g of the desired epoxide product (84%, 1.15 g theoretical). [m/z] = 98. ¹H NMR (CD₃Cl) δ = 3.1 (2H, s), 1.58-1.45 (4H, m), 1.05-0.89 (4H, m). ¹³C NMR (CD₃Cl) δ = 52.09, 24.35, 19.35.

1-Heptene

Caution this reaction is very exothermic

A solution containing $\text{Mn}(\text{CF}_3\text{SO}_3)_2$ (0.0036 g, 1.0×10^{-5} mole), ***R,R*-mcp** (0.0033 g, 1.0×10^{-5} mole), 1-heptene (1.0 g 0.0102 mole), and 12 mL of MeCN was stirred in a 125 mL Erlenmeyer flask at RT until homogeneous. The solution was cooled in an ice bath, and 32% peracetic acid (2.85g, 0.012 mole, 1.2 equivalents) was added via a syringe over the course of 3 minutes. After an additional 10 minutes, the reaction flask was removed from the ice bath and allowed to warm to RT. The solution was carefully diluted with saturated NaHCO_3 (5 mL) and extracted with pentane (3 x 50 mL). The combined organic volume was washed with saturated NaHCO_3 (2 x 50 mL), dried over K_2CO_3 , and filtered through a glass frit. Removal of the solvent under vacuum gave 1.01 g of the desired epoxide product (84%, 1.15 g theoretical). $[\text{m/z}] = 114$. ^1H NMR (CD_3Cl) $\delta = 2.91$ (1H, m), 2.73 (1H, t), 2.45 (1H, q), 1.6-0.9 (11H, m). ^{13}C NMR (CD_3Cl) $\delta = 52.36, 47.08, 32.41, 31.57, 25.6, 22.53, 13.93$.

Cyclooctene

Caution this reaction is very exothermic

A mixture containing $\text{Mn}(\text{CF}_3\text{SO}_3)_2$ (0.0033 g, 9.3×10^{-6} mole), ***R,R*-mcp** (0.003 g, 9.3×10^{-6} mole), cyclooctene (1.03g 0.00936 mole), and 9 mL of MeCN was stirred in a 125 mL Erlenmeyer flask at RT until homogeneous. The solution was cooled in an ice bath, and 32% peracetic acid (2.67g, 0.011 mole, 1.2 equivalents) was added via a syringe over the course of 3 minutes. After an additional 2 minutes, the reaction flask was removed from the ice bath and allowed to warm to RT. The solution was carefully diluted with saturated NaHCO_3 (5 mL) and extracted with pentane (3 x 30 mL). The combined organic volume was washed with saturated NaHCO_3 (2 x 50 mL), dried over K_2CO_3 and filtered through a glass frit. Solvent removal under vacuum gave 1.03 g of cyclooctene oxide (90%, 1.14 g theoretical). $[\text{m/z}] = 126$. ^1H NMR (CD_3Cl) $\delta = 2.89$ (2H, m), 2.16 (2H, m), 1.2-1.7 (10H, m). ^{13}C NMR (CD_3Cl) $\delta = 55.64, 26.52, 26.26, 25.57$.

Quarter-mole scale Epoxidation: Cyclooctene

Caution this reaction is very exothermic

A mixture of $\text{Mn}(\text{CF}_3\text{SO}_3)_2$ (0.088 g, 0.25 mmole), ***R,R*-mcp** (0.080 g, 0.25 mmole), cyclooctene (28.7 g, 0.25 mole), and 250 mL of MeCN was stirred in a 1L flask at RT until homogeneous. The solution was cooled in an ice bath, and 32% peracetic acid (71 g, 0.3 mole, 1.2 equivalents) was added via a drop funnel to a vigorously stirred solution over the course of 5 minutes to insure the temperature did not rise above 25°C . After an additional minute, the flask was removed from the ice bath. The reaction mixture was carefully diluted with 2 g of NaHCO_3 suspended in 100 mL of water and extracted with pentane (3 x 200 mL). The combined organic volume was washed with saturated NaHCO_3 (2 x 100 mL), dried over K_2CO_3 , and filtered through a glass frit. Solvent removal under vacuum gave 27.3 g of cyclooctene oxide (87.5%, 31.2 g theoretical). $[\text{m/z}] = 116$. ^1H NMR (CD_3Cl) $\delta = 2.89$ (2H, m), 2.16 (2H, m), 1.2-1.7 (10H, m). ^{13}C NMR (CD_3Cl) $\delta = 55.64, 26.52, 26.26, 25.57$.

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