Supporting Information for

"A Silica–Gel Supported Ruthenium Complex of 1,4,7-Trimethyl-1,4,7-triazacyclononane as Recyclable Catalyst for Chemoselective Oxidation of Alcohols and Alkenes by *tert*-Butyl Hydroperoxide"

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Experimental for X-ray Crystal Structure Determination

Crystal data: [C₁₇ H₂₄ F₁₂ N₃ O₉ Ru] ; formula weight = 743.46, Monoclinic, P 2₁/n, a = 11.057(2) Å, b = 16.460(3) Å, c = 15.323(3) Å, β = 97.26(3)°, V = 2766.4(10) Å³, Z = 4, D_c = 1.785 g cm⁻³, μ(Mo-Kα) = 0.697 mm⁻¹, F(000) = 1484, T = 301 K.

Data collection: A crystal of dimensions 0.5 x 0.3 x 0.15 mm mounted in a glass capillary was used for data collection at 28°C on a MAR diffractometer with a 300 mm image plate detector using graphite monochromatized Mo-Kα radiation (λ = 0.71073 Å). Data collection was made with 2° oscillation step of φ, 300 seconds exposure time and scanner distance at 120 mm. 100 images were collected.

Data reduction: The images were interpreted and intensities integrated using program DENZO.¹

Structure solution: The structure was solved by direct methods employing SIR-97 program² on PC. Almost all atoms were located according to the direct methods and the successive least-square Fourier cycles. The positions of the other non-hydrogen atoms were found after successful refinement by full-matrix least-squares using program SHELXL-97³ on PC. All the CF₃-groups are disordered into two sets of positions rotating along C-C bonds. Two H atoms on water ligand were located and their positions were fixed in the refinements. Two free CF₃CO₂-fragments were located and one of them should be with proton. O(8) and O(11) are close with distance 2.531 Å, so that a strong hydrogen-bond exists between these two O atoms. Two H atoms on water ligand are also taken part in formation of hydrogen bonds with O atoms of coordinated CF₃CO₂-fragment (O(2)) and free CF₃CO₂-fragment (O(7)).

Structure refinement: According to the SHELXL-97 program³, all 5064 independent reflections (R_{int}⁴ equal to 0.0326, 3942 reflections larger than 4σ(F_o)) from a total 19689 reflections were participated in the full-matrix least-square refinement against F². These reflections were in the range -13 ≤ h ≤ 13, -19 ≤ k ≤ 19, -18 ≤ l ≤ 18 with 2θ_{max} equal to 51.16°.

One crystallographic asymmetric unit consists of one formula unit, including one CF₃CO₂⁻ anion and one CF₃CO₂H. In the final stage of least-squares refinement, all non-H atoms were refined anisotropically. H atoms were generated by program SHELXL-97. The positions of H atoms (except two on water O atom) were calculated based on riding mode with thermal parameters equal to 1.2 times that of the associated C atoms, and participated in the calculation of final R-indices⁵.

¹ Otwinowski, Z. and Minor, W., "Processing of X-ray Diffraction Data Collected in Oscillation Mode", Methods in Enzymology, Volume 276: Macromolecular Crystallography, part A, p. 307-326, 1977. Carter C. W., Sweet Jr. & R. M., Eds., Academic Press.

² A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A.G.G. Moliterni, G. Polidori, R. Spagna. *Sir97: a new tool for crystal structure determination and refinement*. *J. Appl. Cryst.*, **1998**, 32, 115-119.

³ SHELXL97, Sheldrick, G. M. (1997). SHELX97. Programs for Crystal Structure Analysis (Release 97-2). University of Goettingen, Germany.

⁴ $R_{int} = \sum |F_o^2 - F_o^2(\text{mean})| / \sum [F_o^2]$

⁵ Since the structure refinements are against F², R-indices based on F² are larger than (more than double) those based on F. For comparison with older refinements based on F and an OMIT threshold, a conventional index R₁ based on observed F values larger than 4σ(F_o) is also given (corresponding to Intensity ≥ 2σ(I)). $wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$, $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$. The Goodness of Fit is always based on F²: $\text{Goof} = S = \{ \sum [w(F_o^2 - F_c^2)^2] / (n - p) \}^{1/2}$, where n is the number of reflections and p is the total number of parameters refined. The weighting scheme is: $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, where P is $[2 F_c^2 + \text{Max}(F_o^2, 0)]/3$.

Convergence ($(\Delta/\sigma)_{\max} = 0.001$, av. 0.001) for 489 variable parameters by full-matrix least-squares refinement on F^2 reaches to $R_1 = 0.0331$ and $wR_2 = 0.0910$ with a goodness-of-fit of 1.042, the parameters a and b for weighting scheme are 0.0666 and 0.0. The final difference Fourier map shows maximum rest peaks and holes of 0.444 and $-0.557 \text{ e}\text{\AA}^{-3}$ respectively.

Drawing: The ORTEP⁶ drawing of the molecule was made with thermal ellipsoids at the 30 % probability level. Screen drawing is provided for reference. Drawing with high quality can be provided upon request.

Tables: Table (1) of Crystallographic and refinement data, table (2) of atomic coordinates, table (3) of full bond lengths and bond angles and this report⁷ are provided. The other supplementary materials, such as table of anisotropic displacement parameters, table of hydrogen coordinates and/or other tables and/or CIF, RES-files, can be provided under request by notifying the identification code.

⁶ ORTEP3 for Windows - Farrugia, L. J. *J. Appl. Cryst.* 1997, 30, 565.

⁷ The crystallographic data summarised in this reported are abstracted from the previous tables and the experiment record.

Table S1. Crystal data and structure refinement for 1.

Identification code	1	
Empirical formula	C ₁₇ H ₂₄ F ₁₂ N ₃ O ₉ Ru	
Formula weight	743.46	
Temperature	301(2) K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	P 2 ₁ /n	
Unit cell dimensions	a = 11.057(2) Å	α = 90°.
	b = 16.460(3) Å	β = 97.26(3)°.
	c = 15.323(3) Å	γ = 90°.
Volume	2766.4(10) Å ³	
Z	4	
Density (calculated)	1.785 Mg/m ³	
Absorption coefficient	0.697 mm ⁻¹	
F(000)	1484	
Crystal size	0.5 x 0.3 x 0.15 mm ³	
Theta range for data collection	1.82 to 25.58°.	
Index ranges	-13 ≤ h ≤ 13, -19 ≤ k ≤ 19, -18 ≤ l ≤ 18	
Reflections collected	19689	
Independent reflections	5064 [R(int) = 0.0326]	
Completeness to theta = 25.58°	97.3 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5064 / 0 / 489	
Goodness-of-fit on F ²	1.042	
Final R indices [I > 2σ(I)]	R1 = 0.0331, wR2 = 0.0910	
R indices (all data)	R1 = 0.0438, wR2 = 0.1005	
Largest diff. peak and hole	0.444 and -0.557 e.Å ⁻³

Figure S1. Molecular structure of $[(\text{Me}_3\text{tacn})\text{Ru}^{\text{III}}(\text{CF}_3\text{CO}_2)_2(\text{H}_2\text{O})]^+$ (1) complex cation

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Ru(1)	7635(1)	389(1)	7346(1)	45(1)
O(1)	8086(2)	-243(1)	6258(1)	57(1)
O(2)	6777(2)	-1301(2)	6140(2)	70(1)
O(3)	8951(2)	-176(1)	8170(1)	53(1)
O(4)	8805(2)	-1468(1)	7691(2)	68(1)
O(6)	6353(2)	-508(1)	7587(2)	55(1)
O(7)	6938(2)	-1291(2)	9117(2)	71(1)
O(8)	5316(3)	-1166(3)	9828(2)	133(2)
O(9)	4081(5)	-1887(3)	7912(4)	177(2)
O(11)	3923(3)	-679(3)	8492(3)	111(1)
N(1)	8819(2)	1314(2)	7084(2)	57(1)
N(2)	6324(2)	1092(2)	6586(2)	61(1)
N(3)	7278(2)	1141(2)	8380(2)	54(1)
C(1)	8287(4)	1633(2)	6211(2)	71(1)
C(2)	6952(4)	1807(2)	6213(2)	71(1)
C(3)	5506(3)	1355(2)	7246(3)	70(1)
C(4)	6230(3)	1701(2)	8053(2)	68(1)
C(5)	8443(3)	1609(2)	8598(2)	63(1)
C(6)	8861(4)	1961(2)	7786(2)	67(1)
C(7)	10087(3)	1013(2)	7021(3)	71(1)
C(8)	5594(3)	634(2)	5852(3)	77(1)
C(9)	7001(3)	697(2)	9174(2)	64(1)
C(10)	7650(3)	-911(2)	5950(2)	58(1)
C(11)	8321(5)	-1240(3)	5217(3)	83(1)
C(12)	9222(3)	-934(2)	8172(2)	53(1)
C(13)	10233(4)	-1132(2)	8919(3)	74(1)
C(14)	6395(4)	-1314(2)	9765(3)	70(1)
C(15)	7142(5)	-1550(3)	10644(3)	88(1)
C(16)	3715(4)	-1210(3)	7900(4)	102(2)
C(17)	2937(7)	-897(5)	7061(5)	123(2)

F(1')	8310(20)	-709(10)	4616(10)	150(5)
F(1)	7690(16)	-1103(16)	4442(6)	157(8)
F(2)	9317(17)	-850(13)	5113(13)	154(6)
F(2')	9454(12)	-1352(14)	5454(12)	155(7)
F(3)	8530(20)	-2002(6)	5286(12)	153(7)
F(3')	7830(20)	-1861(11)	4845(13)	165(6)
F(4)	11257(11)	-894(12)	8739(11)	152(7)
F(4')	11130(12)	-646(8)	8996(9)	119(6)
F(5)	10033(10)	-758(4)	9672(5)	99(4)
F(5')	9867(10)	-1340(17)	9571(9)	252(11)
F(6')	10859(11)	-1793(8)	8676(10)	164(6)
F(6)	10273(10)	-1894(4)	9129(7)	109(4)
F(7)	7922(11)	-890(5)	10872(6)	118(2)
F(7')	6790(20)	-1286(13)	11306(9)	190(11)
F(8')	8187(12)	-1740(20)	10662(11)	223(11)
F(8)	7845(16)	-2134(8)	10579(8)	136(6)
F(9)	6595(12)	-1660(16)	11306(9)	155(8)
F(9')	6680(20)	-2368(9)	10749(12)	227(7)
F(10)	3380(30)	-1224(17)	6342(17)	250(15)
F(10')	3544(14)	-945(14)	6435(10)	144(5)
F(11')	2694(17)	-123(9)	7152(8)	166(8)
F(11)	3050(30)	-163(13)	6794(18)	279(14)
F(12')	2074(14)	-1408(12)	6932(15)	177(7)
F(12)	1782(14)	-991(15)	7005(12)	190(10)

Table S3. Bond distances [Å] and angles [°] for 1.

Ru(1)-O(3)	2.028(2)	C(11)-F(1)	1.318(11)
Ru(1)-O(1)	2.078(2)	C(12)-C(13)	1.531(5)
Ru(1)-N(1)	2.080(3)	C(13)-F(5')	1.175(11)
Ru(1)-N(3)	2.086(3)	C(13)-F(4)	1.261(15)
Ru(1)-N(2)	2.090(3)	C(13)-F(4')	1.268(13)
Ru(1)-O(6)	2.111(2)	C(13)-F(6)	1.295(9)
O(1)-C(10)	1.268(4)	C(13)-F(5)	1.350(10)
O(2)-C(10)	1.225(4)	C(13)-F(6')	1.366(11)
O(3)-C(12)	1.283(3)	C(14)-C(15)	1.539(6)
O(4)-C(12)	1.201(4)	C(15)-F(8')	1.196(13)
O(7)-C(14)	1.223(4)	C(15)-F(7')	1.213(13)
O(8)-C(14)	1.233(5)	C(15)-F(8)	1.248(10)
O(9)-C(16)	1.184(6)	C(15)-F(9)	1.257(11)
O(11)-C(16)	1.260(6)	C(15)-F(7)	1.404(8)
N(1)-C(1)	1.488(4)	C(15)-F(9')	1.455(12)
N(1)-C(7)	1.501(4)	C(16)-C(17)	1.542(9)
N(1)-C(6)	1.511(4)	C(17)-F(10')	1.240(17)
N(2)-C(8)	1.502(4)	C(17)-F(12')	1.27(2)
N(2)-C(3)	1.504(5)	C(17)-F(12)	1.278(17)
N(2)-C(2)	1.515(5)	C(17)-F(11)	1.29(2)
N(3)-C(9)	1.485(4)	C(17)-F(11')	1.313(16)
N(3)-C(5)	1.502(4)	C(17)-F(10)	1.37(3)
N(3)-C(4)	1.516(4)	F(1')-F(1)	0.960(16)
C(1)-C(2)	1.504(5)	F(1')-F(2)	1.285(19)
C(3)-C(4)	1.497(5)	F(1)-F(3')	1.392(18)
C(5)-C(6)	1.497(5)	F(2)-F(2')	0.979(16)
C(10)-C(11)	1.522(5)	F(2')-F(3)	1.476(19)
C(11)-F(3')	1.259(9)	F(3)-F(3')	0.990(16)
C(11)-F(1')	1.270(13)	F(4)-F(4')	0.60(3)
C(11)-F(2')	1.273(12)	F(4)-F(6')	1.54(2)
C(11)-F(3)	1.278(9)	F(4')-F(5)	1.701(19)
C(11)-F(2)	1.302(13)	F(5)-F(5')	0.98(3)

F(5')-F(6)	1.25(2)	C(7)-N(1)-Ru(1)	112.78(19)
F(6')-F(6)	1.021(13)	C(6)-N(1)-Ru(1)	110.0(2)
F(7)-F(8')	1.48(3)	C(8)-N(2)-C(3)	109.6(3)
F(7)-F(7')	1.63(2)	C(8)-N(2)-C(2)	109.7(3)
F(7')-F(9)	0.65(3)	C(3)-N(2)-C(2)	111.9(3)
F(8')-F(8)	0.75(3)	C(8)-N(2)-Ru(1)	114.1(2)
F(8)-F(9')	1.397(19)	C(3)-N(2)-Ru(1)	102.61(19)
F(9)-F(9')	1.455(19)	C(2)-N(2)-Ru(1)	108.8(2)
F(10)-F(10')	0.51(4)	C(9)-N(3)-C(5)	109.3(3)
F(10')-F(11)	1.53(3)	C(9)-N(3)-C(4)	109.9(3)
F(11')-F(11)	0.72(4)	C(5)-N(3)-C(4)	111.1(3)
F(11')-F(12)	1.75(3)	C(9)-N(3)-Ru(1)	114.20(19)
F(12')-F(12)	0.77(3)	C(5)-N(3)-Ru(1)	103.56(19)
		C(4)-N(3)-Ru(1)	108.66(19)
O(3)-Ru(1)-O(1)	92.54(9)	N(1)-C(1)-C(2)	110.1(3)
O(3)-Ru(1)-N(1)	92.04(9)	C(1)-C(2)-N(2)	110.4(3)
O(1)-Ru(1)-N(1)	89.44(10)	C(4)-C(3)-N(2)	111.1(3)
O(3)-Ru(1)-N(3)	89.34(9)	C(3)-C(4)-N(3)	110.4(3)
O(1)-Ru(1)-N(3)	173.29(9)	C(6)-C(5)-N(3)	111.1(3)
N(1)-Ru(1)-N(3)	84.05(11)	C(5)-C(6)-N(1)	109.5(3)
O(3)-Ru(1)-N(2)	173.29(9)	O(2)-C(10)-O(1)	129.9(3)
O(1)-Ru(1)-N(2)	92.86(10)	O(2)-C(10)-C(11)	117.4(3)
N(1)-Ru(1)-N(2)	84.03(11)	O(1)-C(10)-C(11)	112.6(3)
N(3)-Ru(1)-N(2)	84.86(10)	F(3')-C(11)-F(1')	105.5(9)
O(3)-Ru(1)-O(6)	90.89(8)	F(3')-C(11)-F(2')	111.3(10)
O(1)-Ru(1)-O(6)	91.48(9)	F(1')-C(11)-F(2')	102.8(11)
N(1)-Ru(1)-O(6)	176.89(9)	F(3')-C(11)-F(3)	46.0(8)
N(3)-Ru(1)-O(6)	94.93(10)	F(1')-C(11)-F(3)	136.1(8)
N(2)-Ru(1)-O(6)	92.95(10)	F(2')-C(11)-F(3)	70.7(9)
C(10)-O(1)-Ru(1)	127.8(2)	F(3')-C(11)-F(2)	131.9(8)
C(12)-O(3)-Ru(1)	126.56(18)	F(1')-C(11)-F(2)	59.9(9)
C(1)-N(1)-C(7)	109.0(3)	F(2')-C(11)-F(2)	44.7(8)
C(1)-N(1)-C(6)	111.3(3)	F(3)-C(11)-F(2)	110.1(9)
C(7)-N(1)-C(6)	109.5(3)	F(3')-C(11)-F(1)	65.3(8)
C(1)-N(1)-Ru(1)	104.17(19)	F(1')-C(11)-F(1)	43.5(8)

F(2')-C(11)-F(1)	132.1(10)	O(8)-C(14)-C(15)	113.5(4)
F(3)-C(11)-F(1)	108.3(10)	F(8')-C(15)-F(7')	119.3(13)
F(2)-C(11)-F(1)	99.5(10)	F(8')-C(15)-F(8)	35.7(13)
F(3')-C(11)-C(10)	113.7(7)	F(7')-C(15)-F(8)	127.8(11)
F(1')-C(11)-C(10)	109.4(7)	F(8')-C(15)-F(9)	120.3(10)
F(2')-C(11)-C(10)	113.3(7)	F(7')-C(15)-F(9)	30.4(13)
F(3)-C(11)-C(10)	113.0(6)	F(8)-C(15)-F(9)	108.8(11)
F(2)-C(11)-C(10)	114.4(6)	F(8')-C(15)-F(7)	68.7(13)
F(1)-C(11)-C(10)	110.6(7)	F(7')-C(15)-F(7)	76.6(11)
O(4)-C(12)-O(3)	129.7(3)	F(8)-C(15)-F(7)	104.2(9)
O(4)-C(12)-C(13)	119.4(3)	F(9)-C(15)-F(7)	104.7(10)
O(3)-C(12)-C(13)	110.9(3)	F(8')-C(15)-F(9')	95.9(13)
F(5')-C(13)-F(4)	133.8(9)	F(7')-C(15)-F(9')	94.8(12)
F(5')-C(13)-F(4')	117.0(12)	F(8)-C(15)-F(9')	61.7(10)
F(4)-C(13)-F(4')	27.3(12)	F(9)-C(15)-F(9')	64.4(10)
F(5')-C(13)-F(6)	60.7(11)	F(7)-C(15)-F(9')	154.2(7)
F(4)-C(13)-F(6)	110.6(10)	F(8')-C(15)-C(14)	119.8(8)
F(4')-C(13)-F(6)	125.9(7)	F(7')-C(15)-C(14)	116.6(10)
F(5')-C(13)-F(5)	45.2(13)	F(8)-C(15)-C(14)	113.3(7)
F(4)-C(13)-F(5)	107.1(9)	F(9)-C(15)-C(14)	118.9(8)
F(4')-C(13)-F(5)	81.0(9)	F(7)-C(15)-C(14)	105.5(5)
F(6)-C(13)-F(5)	103.5(8)	F(9')-C(15)-C(14)	100.1(6)
F(5')-C(13)-F(6')	103.9(12)	O(9)-C(16)-O(11)	127.6(7)
F(4)-C(13)-F(6')	71.8(9)	O(9)-C(16)-C(17)	118.7(6)
F(4')-C(13)-F(6')	96.3(8)	O(11)-C(16)-C(17)	113.6(5)
F(6)-C(13)-F(6')	45.0(6)	F(10')-C(17)-F(12')	107.9(14)
F(5)-C(13)-F(6')	137.6(7)	F(10')-C(17)-F(12)	125.0(12)
F(5')-C(13)-C(12)	113.6(6)	F(12')-C(17)-F(12)	35.3(12)
F(4)-C(13)-C(12)	111.2(8)	F(10')-C(17)-F(11)	74.3(19)
F(4')-C(13)-C(12)	115.1(6)	F(12')-C(17)-F(11)	132.4(15)
F(6)-C(13)-C(12)	113.0(4)	F(12)-C(17)-F(11)	103.1(17)
F(5)-C(13)-C(12)	111.1(5)	F(10')-C(17)-F(11')	106.3(15)
F(6')-C(13)-C(12)	108.3(6)	F(12')-C(17)-F(11')	119.9(12)
O(7)-C(14)-O(8)	129.5(4)	F(12)-C(17)-F(11')	84.7(13)
O(7)-C(14)-C(15)	117.0(4)	F(11)-C(17)-F(11')	32.0(19)

F(10')-C(17)-F(10)	21.7(19)	F(5')-F(5)-C(13)	58.0(9)
F(12')-C(17)-F(10)	87.3(15)	F(5')-F(5)-F(4')	98.3(13)
F(12)-C(17)-F(10)	110.8(16)	C(13)-F(5)-F(4')	47.4(6)
F(11)-C(17)-F(10)	93.1(19)	F(5)-F(5')-C(13)	76.8(14)
F(11')-C(17)-F(10)	124.4(16)	F(5)-F(5')-F(6)	136.1(17)
F(10')-C(17)-C(16)	108.9(9)	C(13)-F(5')-F(6)	64.4(9)
F(12')-C(17)-C(16)	103.7(12)	F(6)-F(6')-C(13)	63.8(8)
F(12)-C(17)-C(16)	117.6(11)	F(6)-F(6')-F(4)	108.4(13)
F(11)-C(17)-C(16)	120.8(11)	C(13)-F(6')-F(4)	50.9(7)
F(11')-C(17)-C(16)	109.6(7)	F(6')-F(6)-F(5')	123.4(14)
F(10)-C(17)-C(16)	108.7(15)	F(6')-F(6)-C(13)	71.2(9)
F(1)-F(1')-C(11)	70.9(14)	F(5')-F(6)-C(13)	54.9(7)
F(1)-F(1')-F(2)	125(2)	C(15)-F(7)-F(8')	49.0(6)
C(11)-F(1')-F(2)	61.3(9)	C(15)-F(7)-F(7')	46.4(5)
F(1')-F(1)-C(11)	65.6(11)	F(8')-F(7)-F(7')	83.9(9)
F(1')-F(1)-F(3')	116.5(18)	F(9)-F(7')-C(15)	78.5(18)
C(11)-F(1)-F(3')	55.3(7)	F(9)-F(7')-F(7)	130(3)
F(2')-F(2)-F(1')	122(2)	C(15)-F(7')-F(7)	56.9(9)
F(2')-F(2)-C(11)	66.1(13)	F(8)-F(8')-C(15)	76.0(16)
F(1')-F(2)-C(11)	58.8(9)	F(8)-F(8')-F(7)	138(2)
F(2)-F(2')-C(11)	69.2(12)	C(15)-F(8')-F(7)	62.3(11)
F(2)-F(2')-F(3)	117.5(19)	F(8')-F(8)-C(15)	68.4(15)
C(11)-F(2')-F(3)	54.8(7)	F(8')-F(8)-F(9')	131(2)
F(3')-F(3)-C(11)	66.0(8)	C(15)-F(8)-F(9')	66.4(8)
F(3')-F(3)-F(2')	114.4(13)	F(7')-F(9)-C(15)	71.1(17)
C(11)-F(3)-F(2')	54.5(6)	F(7')-F(9)-F(9')	135(2)
F(3)-F(3')-C(11)	68.0(9)	C(15)-F(9)-F(9')	64.4(8)
F(3)-F(3')-F(1)	123.1(14)	F(8)-F(9')-C(15)	51.9(6)
C(11)-F(3')-F(1)	59.4(6)	F(8)-F(9')-F(9)	91.1(9)
F(4')-F(4)-C(13)	77(2)	C(15)-F(9')-F(9)	51.2(6)
F(4')-F(4)-F(6')	127(3)	F(10')-F(10)-C(17)	65(4)
C(13)-F(4)-F(6')	57.3(8)	F(10)-F(10')-C(17)	94(5)
F(4)-F(4')-C(13)	76(2)	F(10)-F(10')-F(11)	137(5)
F(4)-F(4')-F(5)	125(3)	C(17)-F(10')-F(11)	54.3(13)
C(13)-F(4')-F(5)	51.6(6)	F(11)-F(11')-C(17)	72(2)

F(11)-F(11')-F(12)	101(3)
C(17)-F(11')-F(12)	46.8(8)
F(11')-F(11)-C(17)	76(3)
F(11')-F(11)-F(10')	127(3)
C(17)-F(11)-F(10')	51.4(12)
F(12)-F(12')-C(17)	73(3)
F(12')-F(12)-C(17)	72(2)
F(12')-F(12)-F(11')	120(3)
C(17)-F(12)-F(11')	48.5(9)

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**. The anisotropicdisplacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	57(1)	38(1)	43(1)	0(1)	11(1)	0(1)
O(1)	76(1)	48(1)	48(1)	-2(1)	19(1)	0(1)
O(2)	85(2)	65(2)	63(2)	-14(1)	16(1)	-14(1)
O(3)	61(1)	42(1)	56(1)	-1(1)	8(1)	1(1)
O(4)	88(2)	46(1)	67(2)	-6(1)	1(1)	2(1)
O(6)	62(1)	51(1)	56(1)	-1(1)	18(1)	-5(1)
O(7)	81(2)	71(2)	63(2)	10(1)	25(1)	2(1)
O(8)	87(2)	227(5)	92(2)	12(3)	33(2)	29(2)
O(9)	164(4)	100(3)	264(6)	-22(4)	20(4)	37(3)
O(11)	86(2)	133(3)	120(3)	-20(2)	32(2)	16(2)
N(1)	72(2)	43(1)	58(2)	2(1)	20(1)	-4(1)
N(2)	72(2)	54(2)	55(2)	4(1)	5(1)	9(1)
N(3)	68(2)	45(1)	50(1)	-2(1)	15(1)	4(1)
C(1)	100(3)	51(2)	64(2)	11(2)	23(2)	-3(2)
C(2)	105(3)	51(2)	57(2)	12(2)	10(2)	7(2)
C(3)	69(2)	67(2)	75(2)	2(2)	10(2)	16(2)
C(4)	78(2)	58(2)	71(2)	-1(2)	20(2)	17(2)
C(5)	81(2)	49(2)	61(2)	-11(2)	11(2)	-9(2)
C(6)	85(2)	46(2)	70(2)	-9(2)	20(2)	-13(2)
C(7)	70(2)	68(2)	80(2)	1(2)	27(2)	-8(2)
C(8)	83(2)	78(2)	66(2)	-3(2)	-13(2)	8(2)
C(9)	88(2)	58(2)	50(2)	-2(2)	24(2)	1(2)
C(10)	79(2)	51(2)	43(2)	-2(1)	9(2)	7(2)
C(11)	110(4)	79(3)	67(3)	-10(2)	35(2)	-2(3)
C(12)	57(2)	46(2)	56(2)	5(1)	11(1)	1(1)
C(13)	67(2)	60(2)	90(3)	8(2)	-6(2)	4(2)
C(14)	79(2)	60(2)	74(3)	-3(2)	22(2)	0(2)
C(15)	106(4)	97(3)	65(3)	4(2)	25(2)	12(3)
C(16)	78(3)	100(4)	134(5)	-21(3)	39(3)	2(3)

C(17)	114(5)	143(6)	114(5)	-25(5)	18(4)	-17(5)
F(1')	221(19)	164(10)	79(9)	15(8)	78(9)	24(12)
F(1)	160(11)	270(20)	40(3)	-11(8)	5(5)	58(11)
F(2)	147(12)	176(14)	162(16)	-70(10)	105(12)	-31(10)
F(2')	103(6)	213(18)	148(10)	-76(10)	17(6)	66(10)
F(3)	268(19)	71(5)	144(10)	20(6)	125(10)	74(10)
F(3')	240(15)	133(10)	138(12)	-100(9)	88(9)	-70(10)
F(4)	52(4)	270(20)	135(9)	-3(10)	15(4)	-23(8)
F(4')	104(9)	103(5)	133(11)	12(6)	-57(9)	-19(4)
F(5)	128(8)	109(4)	51(4)	-16(4)	-17(4)	37(5)
F(5')	101(6)	530(30)	115(12)	178(18)	-9(8)	-9(19)
F(6')	118(8)	121(8)	237(14)	-19(8)	-40(7)	60(7)
F(6)	125(9)	51(3)	134(9)	10(4)	-50(7)	6(4)
F(7)	135(6)	111(5)	100(5)	-21(4)	-15(5)	-32(4)
F(7')	270(20)	227(16)	67(8)	-63(10)	-3(8)	97(14)
F(8')	85(5)	470(30)	111(10)	98(17)	16(5)	55(13)
F(8)	209(16)	113(6)	83(5)	-2(5)	9(8)	98(9)
F(9)	118(6)	280(20)	81(8)	64(11)	54(5)	20(9)
F(9')	330(20)	172(12)	164(12)	84(10)	-18(12)	-52(12)
F(10)	370(30)	230(20)	171(14)	-95(11)	97(14)	-75(15)
F(10')	153(8)	188(16)	99(7)	-29(8)	51(6)	-21(9)
F(11')	239(16)	133(10)	107(6)	-17(6)	-52(7)	105(12)
F(11)	340(20)	172(18)	300(30)	73(19)	-60(20)	-66(16)
F(12')	103(10)	220(14)	197(12)	-65(11)	-15(9)	-18(9)
F(12)	75(6)	340(30)	149(10)	38(16)	4(5)	11(11)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(1A)	8392	1237	5758	85
H(1B)	8707	2127	6080	85
H(2A)	6577	1914	5617	85
H(2B)	6854	2288	6564	85
H(3A)	4938	1762	6983	84
H(3B)	5039	893	7409	84
H(4A)	5706	1771	8510	82
H(4B)	6546	2230	7919	82
H(5A)	8317	2044	9004	76
H(5B)	9070	1252	8884	76
H(6A)	9687	2165	7920	80
H(6B)	8338	2411	7575	80
H(7A)	10437	806	7582	107
H(7B)	10578	1453	6851	107
H(7C)	10057	589	6589	107
H(8A)	5211	174	6089	116
H(8B)	6123	450	5442	116
H(8C)	4980	984	5556	116
H(9A)	6251	402	9039	96
H(9B)	6921	1079	9638	96
H(9C)	7650	324	9360	96
H(1)	6444	-882	8133	109(14)
H(2)	6534	-860	7185	98(14)

Hydrogen bonds with $H \cdots A < r(A) + 2.200$ Angstroms and $\angle DHA > 110$ deg.

D-H	d(D-H)	d(H...A)	$\angle DHA$	d(D...A)	A
O6-H1	1.033	1.679	162.46	2.682	O7
O6-H2	0.888	1.810	161.62	2.667	O2
O6-H2	0.888	2.572	110.50	3.000	O1

Figure S2. The solid diffuse-reflectance UV-vis spectrum of unloaded silica gel

Figure S3. The solid diffuse-reflectance UV-vis spectrum of 1-SiO₂

Figure S4. The solid diffuse-reflectance UV-vis spectrum of the recovered 1-SiO₂ catalyst with CH₂Cl₂ as solvent for oxidation