

Supporting Information

Aerial oxidation of tetrahydrofuran to 2-hydroxotetrahydrofuran in the presence of a trimeric Cu^I complex [Cu₃L₃] (HL = *t*BuNHC(S)NHP(S)(*Oi*Pr)₂) and trapping of the unstable product at recrystallization

Robert C. Luckay,^a Xia Sheng,^a Christoph E. Strasser,^a Helgard G. Raubenheimer,^a
Damir A. Safin,^{*b} Maria G. Babashkina,^b and Axel Klein^{*b}

^a Department of Chemistry, University of Stellenbosch, Private Bag X1, MATIELAND 7602, Stellenbosch, South Africa

^b Institut für Anorganische Chemie, Universität zu Köln, Greinstrasse 6, D-50939 Köln, Germany

E-mail: damir.safin@ksu.ru (D. A. Safin), axel.klein@uni-koeln.de (A. Klein)

Table S1. Product selectivity in the oxidation of THF

N	Sample	2-hydroxotetrahydrofuran (yield, %)							
		1 h	6 h	10 h	24 h	36 h	48 h	60 h	72 h
1	THF	0.05±0.01							
2	THF (O ₂)	0.8±0.1	1.0±0.12	1.2±0.1	1.8±0.1	1.9±0.14	1.9±0.1	2.0±0.15	2.2±0.2
3	THF (O ₂ + UV)	0.8±0.12	1.1±0.1	1.4±0.15	1.9±0.1	1.9±0.16	2.0±0.1	2.2±0.17	2.3±0.1
4	THF + [Cu ₃ L ₃] (Ar)	1.0±0.12	1.0±0.11	1.1±0.1	1.3±0.12	1.3±0.1	1.4±0.12	1.4±0.14	1.4±0.12
5	THF + [Cu ₃ L ₃] (Ar + UV)	1.1±0.11	1.2±0.08	1.3±0.09	1.3±0.1	1.3±0.06	1.4±0.1	1.5±0.14	1.6±0.08
6	THF + [Cu ₃ L ₃] (O ₂)	2.5±0.12	4.3±0.14	7.6±0.1	13.9±0.14	17.9±0.12	22.5±0.12	23.8±0.1	24.1±0.14
7	THF + [Cu ₃ L ₃] (O ₂ + UV)	2.8±0.08	4.7±0.1	8.0±0.12	15.7±0.1	19.6±0.06	24.2±0.18	24.9±0.15	25.2±0.12

Table S1 (continuation). Product selectivity in the oxidation of THF

N	Sample	4-butyrolactone (yield, %)							
		1 h	6 h	10 h	24 h	36 h	48 h	60 h	72 h
1	THF								
2	THF (O ₂)	0.3±0.06	0.5±0.08	0.7±0.1	1.1±0.14	1.2±0.1	1.2±0.14	1.3±0.12	1.4±0.08
3	THF (O ₂ + UV)	0.7±0.1	0.9±0.1	1.3±0.18	1.9±0.2	1.9±0.15	2.0±0.12	2.0±0.08	2.1±0.1
4	THF + [Cu ₃ L ₃] (Ar)	0.8±0.08	0.8±0.12	1.0±0.1	1.0±0.08	1.1±0.12	1.2±0.08	1.2±0.1	1.3±0.07
5	THF + [Cu ₃ L ₃] (Ar + UV)	0.9±0.12	1.0±0.06	1.0±0.14	1.1±0.07	1.1±0.1	1.3±0.12	1.3±0.06	1.4±0.1
6	THF + [Cu ₃ L ₃] (O ₂)	1.1±0.14	1.1±0.1	1.3±0.16	1.6±0.12	1.8±0.18	2.0±0.18	2.1±0.07	2.4±0.18
7	THF + [Cu ₃ L ₃] (O ₂ + UV)	0.9±0.08	1.0±0.12	1.3±0.1	1.7±0.18	1.9±0.15	2.2±0.2	2.4±0.1	2.6±0.1

Table S1 (continuation). Product selectivity in the oxidation of THF

N	Sample	2,3-dihydrofuran (yield, %)						
		6 h	10 h	24 h	36 h	48 h	60 h	72 h
1	THF							
2	THF (O ₂)							
3	THF (O ₂ + UV)							
4	THF + [Cu ₃ L ₃] (Ar)							
5	THF + [Cu ₃ L ₃] (Ar + UV)							
6	THF + [Cu ₃ L ₃] (O ₂)		3.7±0.08	5.9±0.1	5.9±0.07	6.3±0.08	6.6±0.12	6.7±0.14
7	THF + [Cu ₃ L ₃] (O ₂ + UV)	0.4±0.06	4.0±0.1	6.2±0.14	6.4±0.12	6.5±0.1	6.9±0.15	7.4±0.1