

Electronic Supplementary Information

For “Diruthenium(II,III) tetramidates as a new class of oxygenation catalysts”

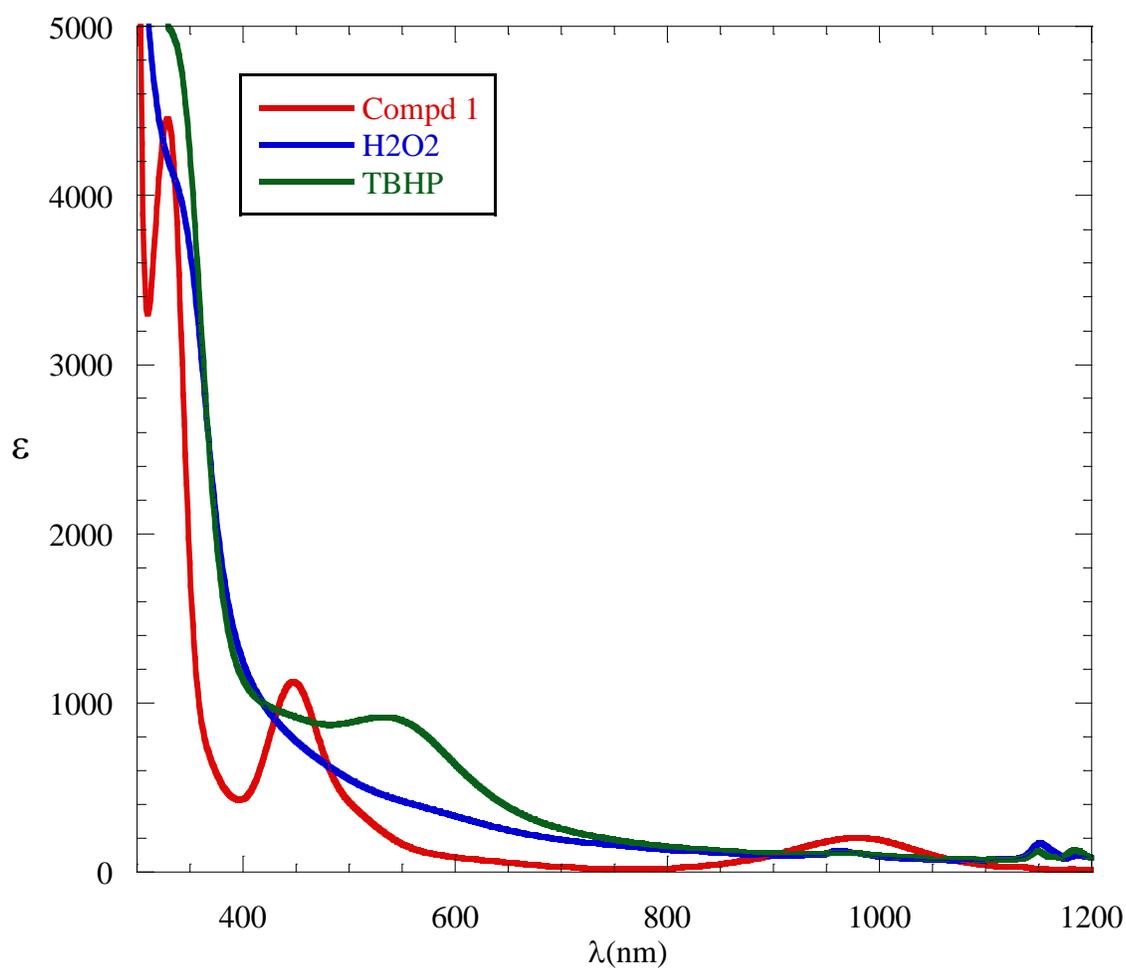


Figure S1. Vis-NIR spectra of compound **1** and its degradation products recorded in CH_3CN . The “ H_2O_2 ” and “TBHP” spectra were recorded after **1** was reacted with 8 equiv of H_2O_2 and TBHP in CH_3CN 24 h, respectively.

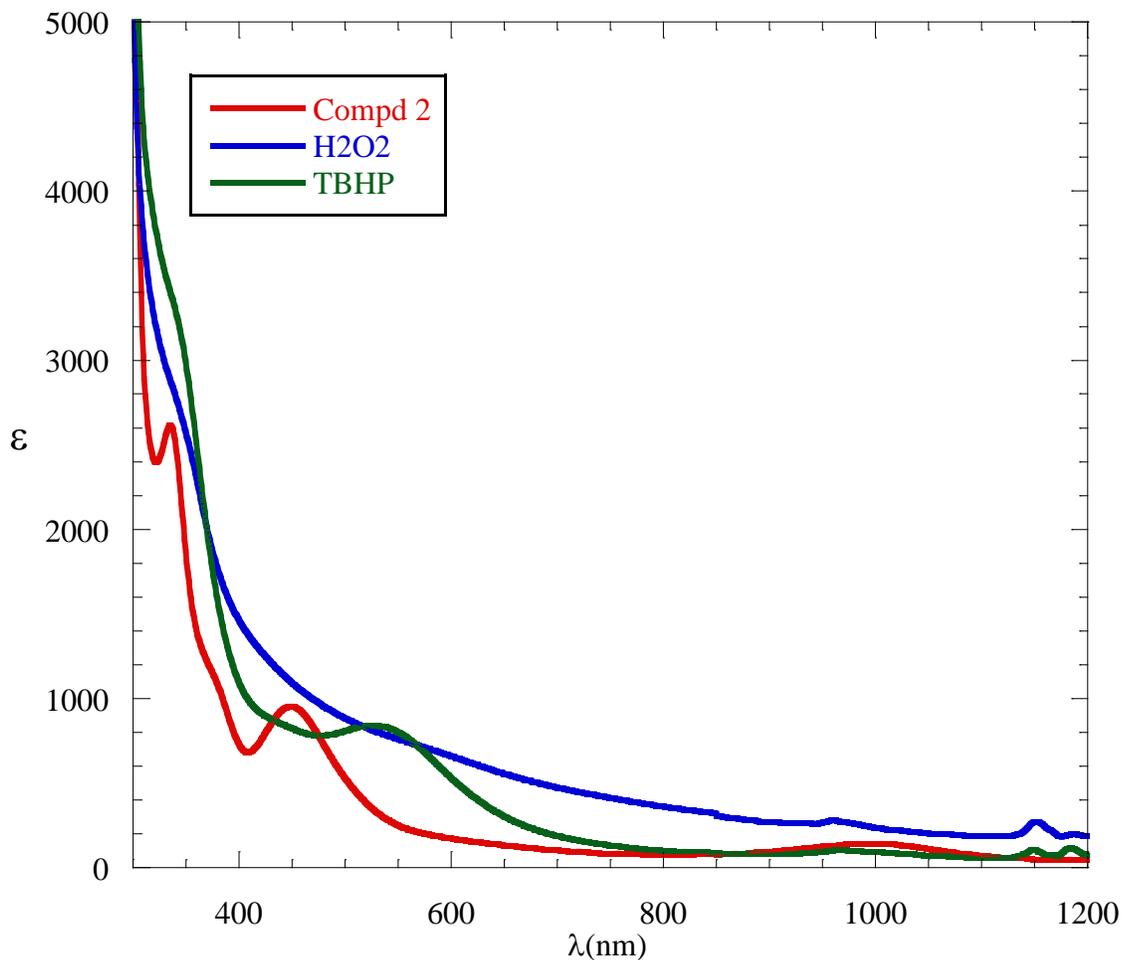


Figure S2. Vis-NIR spectra of compound **2** and its degradation products recorded in CH_3CN . The “ H_2O_2 ” and “TBHP” spectra were recorded after **2** was reacted with 8 equiv of H_2O_2 and TBHP in CH_3CN for 24 h, respectively.

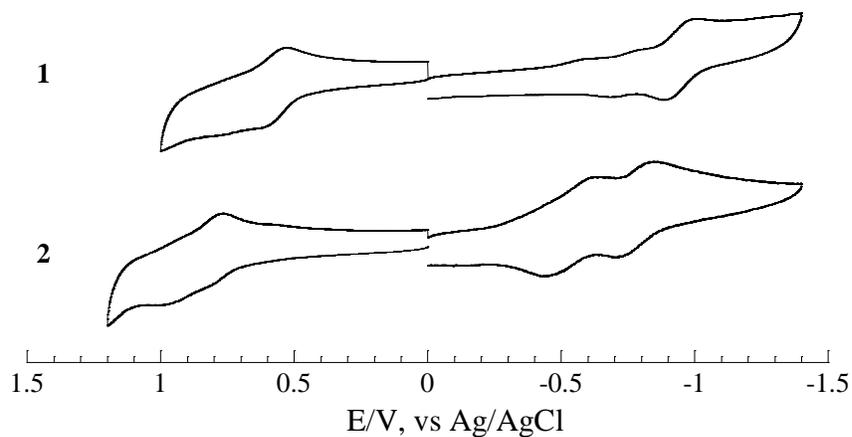


Figure S3. Cyclic voltammograms of compounds **1** and **2** recorded in CH_3CN .

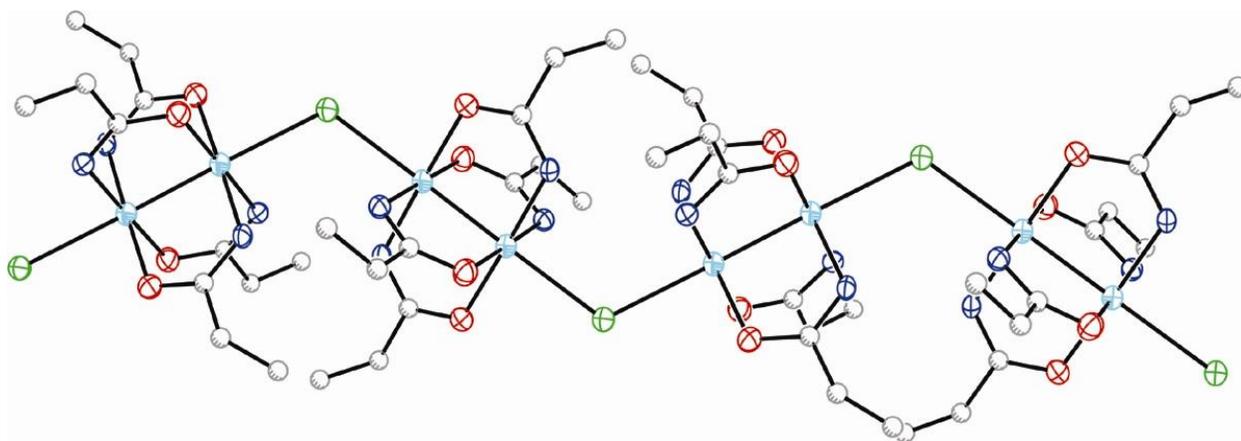


Figure S4. The chain structure of compound 2.

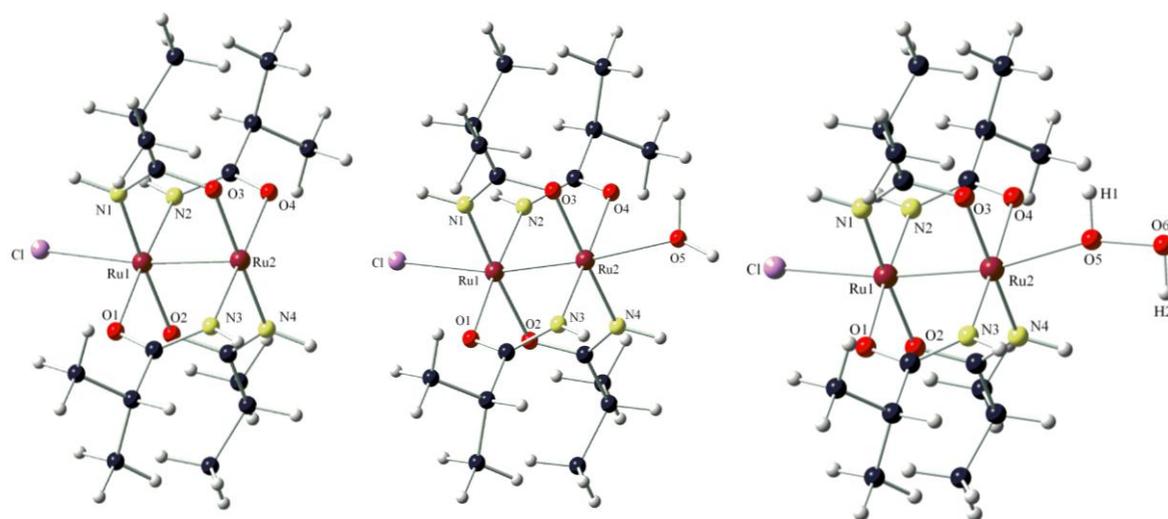


Figure S5. The optimized structures of **1'** (left), **1'•H₂O** and **1'•H₂O₂** (right).

Table S1. Optimized Bond Lengths (Å) and Angles (deg) Computed for **1'**, **1'•H₂O** and **1'•H₂O₂**

	1'	1'•H₂O	1'•H₂O₂
Ru1-Ru2	2.355	2.375	2.388
Ru1-Cl	2.483	2.525	2.494
Ru1-N1	2.049	2.039	2.037
Ru1-N2	2.049	2.039	2.037
Ru1-O1	2.093	2.090	2.089
Ru1-O2	2.093	2.090	2.089
Ru2-N3	2.049	2.039	2.037
Ru2-N4	2.049	2.039	2.037
Ru2-O3	2.066	2.088	2.089
Ru2-O4	2.066	2.088	2.089
Ru2-O5		2.448	2.314
O5-O6			1.618
Ru2-Ru1-Cl	172.5	170.3	172.2
Ru2-Ru1-O5		174.5	168.4
Ru2-O5-O6			160.7
Ru2-Ru1-N1	86.9	86.5	87.1
Ru2-Ru1-N2	86.9	86.5	87.1
Ru2-Ru1-O1	89.6	90.3	89.7
Ru2-Ru1-O2	89.6	90.3	89.7
Ru1-Ru2-N3	88.6	87.9	88.2
Ru1-Ru2-N4	88.6	87.9	88.2
Ru1-Ru2-O3	91.2	91.6	90.7
Ru1-Ru2-O4	91.2	91.6	90.7