Supplementary Material (ESI) for Dalton Transactions

Electronic Supporting Information (ESI)

Kinetics and mechanism of O-O bond cleavage in the reaction of $[Ru^{III}(edta)(H_2O)]^-$ with hydroperoxides in aqueous solution

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Table S1 Effect of the $KHSO_5$/^{t}BuOOH concentration on k'_{obs} for the formation of $ABTS^{\bullet+}$ at 25 °C. $[Ru^{III}(edta)] = 1 \times 10^{-6}$ M, [ABTS] = 1×10^{-3} M, pH = 6.1 (0.2 M acetate buffer).

[POH], (M)	k'_{obs}, (s^{-1})	
	$KHSO_5$	^{t}BuOOH
0.0025	0.011 ± 0.002	0.004 ± 0.0002
0.005	0.017 ± 0.003	0.008 ± 0.0003
0.0075	0.02 ± 0.004	0.012 ± 0.003
0.01	0.022 ± 0.042	0.015 ± 0.003
0.0125	0.024 ± 0.003	0.019 ± 0.004

For the rate constants that are directly obtained from the slope, the uncertainty was taken as it was obtained by linear fit using Origin 6.0 program. In other cases the uncertainty calculation was carried out as per following example:

A = 1.67 ± 0.05; B = 5.23 ± 0.09 and C = 1.88 ± 0.07. Now to compute standard deviation (dx) for X = (A x B)/C, we proceed as follows. Here, X = (1.67 x 5.23)/1.88 = **4.65**

Now $dx/4.65 = \{(0.05/1.67)^2 + (0.09/5.23)^2 + (0.07/1.88)^2\}^{1/2} = 0.508$

$dx = 4.65 \times 0.508 = 0.235$.

So, the value of X with standard deviation would be **4.65 ± 0.23**

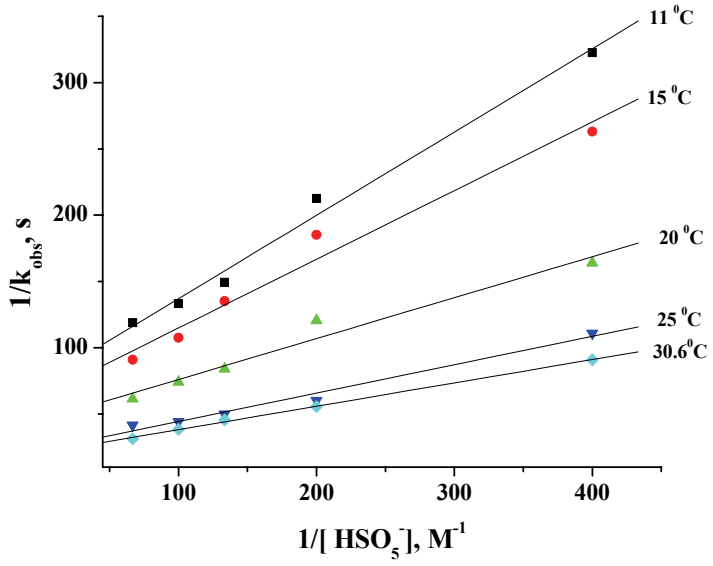

Figure S1. Plot of $1/k_{obs}$ *vs.* $1/[HSO_5^-]$ for the reaction between $[Ru(edta)H_2O]^-$ (1.0×10^{-4} M) and $KHSO_5$ at different temperatures and pH = 6.0 (0.2 M acetate buffer), followed at 391 nm.

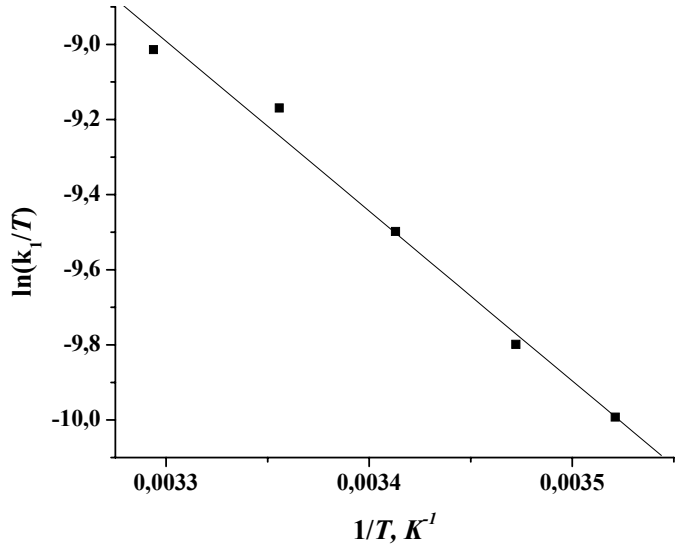

Figure S2. Eyring plot of $\ln(k_1/T)$ versus $1/T$ for the data in Table 1: $[Ru^{III}] = 1 \times 10^{-4}$ M, pH = 6.1 (0.2 M acetate buffer).

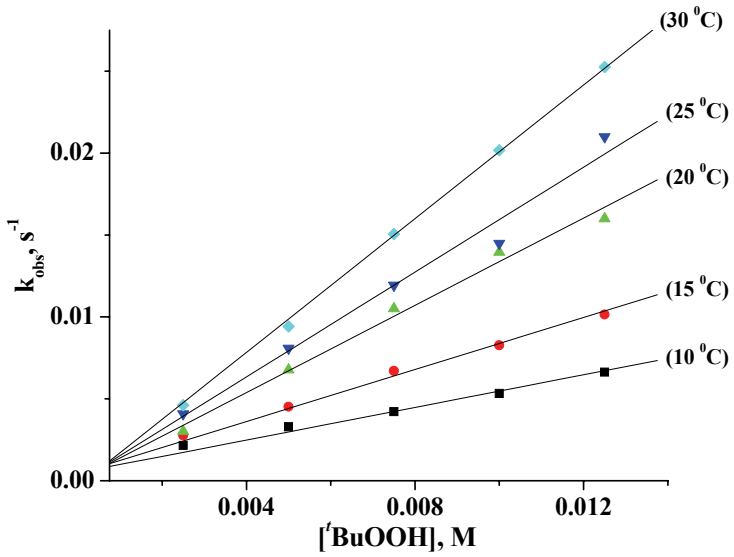

Figure S3. Plot of k_{obs} *vs.* [^{t}BuOOH] for the reaction between $[Ru(edta)H_2O]^-$ (1.0×10^{-4} M) and ^{t}BuOOH at different temperatures and pH = 6.0 (0.2 M acetate buffer).