Supplementary Information

A Non-heme Cationic Fe^{3+}-complex Intercalated in Montmorillonite K-10: Synthesis, Characterization and Catalytic Alkane Hydroxylation with H_2O_2 at Room Temperature

Anand Pariyar,[a] Suranjana Bose,[a] Achintesh Narayan Biswas,[b] Sudip Barman,[c] Pinaki Bandyopadhyay*[a]

[a]Department of Chemistry, University of North Bengal, Siliguri 734013, West Bengal, India.

[b]Department of Chemistry, Siliguri College, Siliguri 734001, West Bengal, India.

[c] School of Chemical Science, National Institute of Science Education and Research (NISER), Bhubaneswar, Orissa 751005, India.

*Email: chempb@gmail.com

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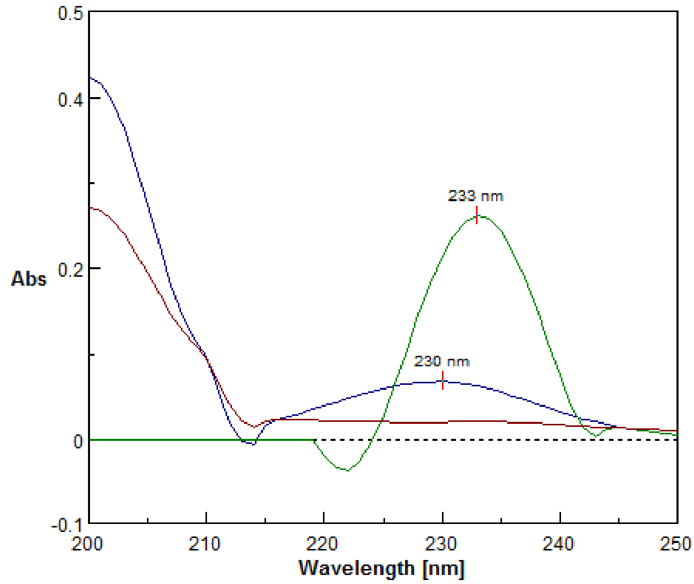

Figure S1. Solid state uv-visible spectra of **1 (green)**, **Mont (red)** and **1-Mont (blue)** in KBr disc. The curve was obtained using Savitzky-Golay alogtithm with 1st order of derivative over 25 data points with 3rd order polynomial fit.

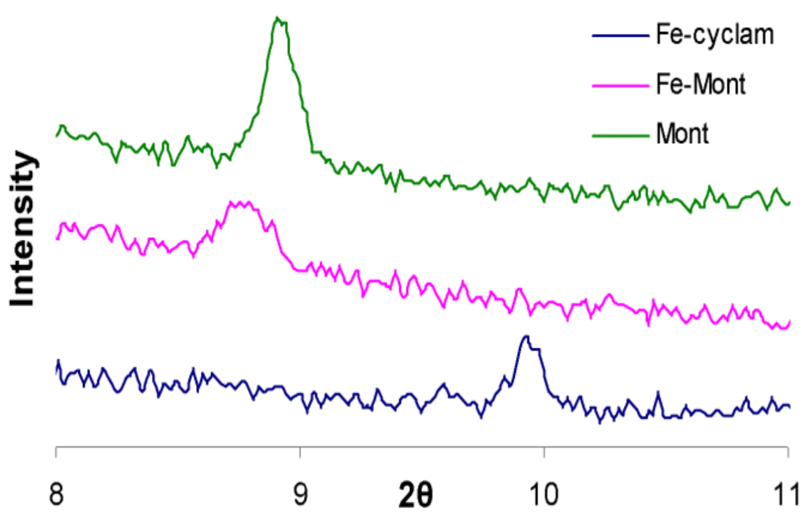

Figure S2. PXRD pattern of **Montmorilonite K-10 (Mont)**, **1(Fe-cyclam)** and **1-Mont (Fe-Mont)** at small angle.

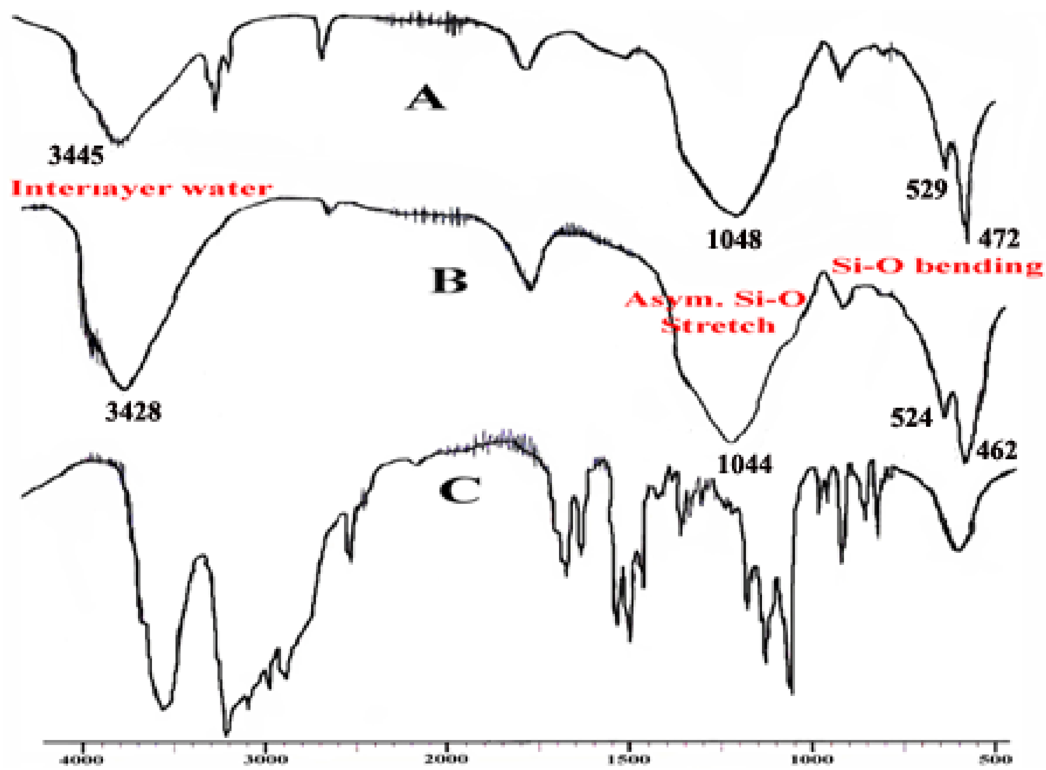

Figure S3. FT-IR spectra of **1-Mont (A)**, **Montmorollonite K-10(B)**, and **1 (C)** in KBr disc.

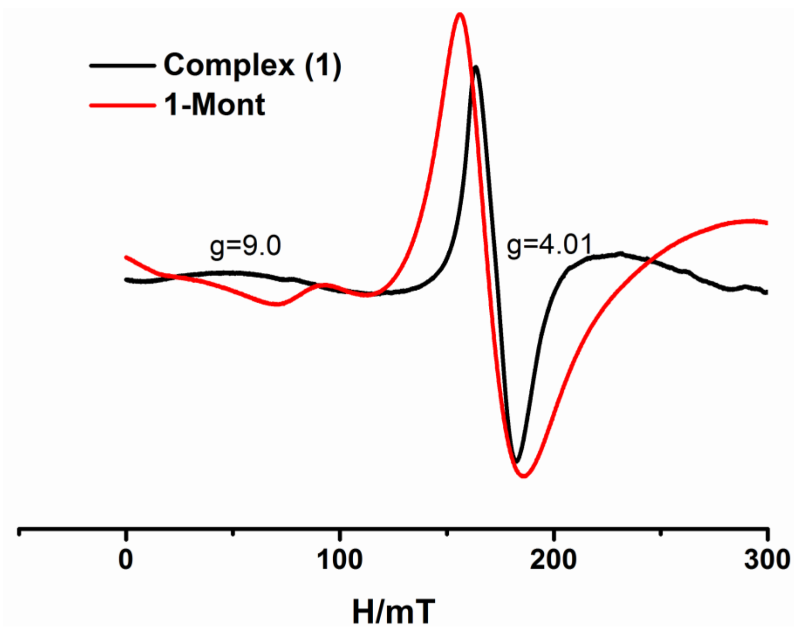

Figure S4. X-band EPR spectra recorded in the solid state at 77K of *cis*-[Fe^{III}(cyclam)Cl_2]Cl (black line) and **1-Mont** (red line).

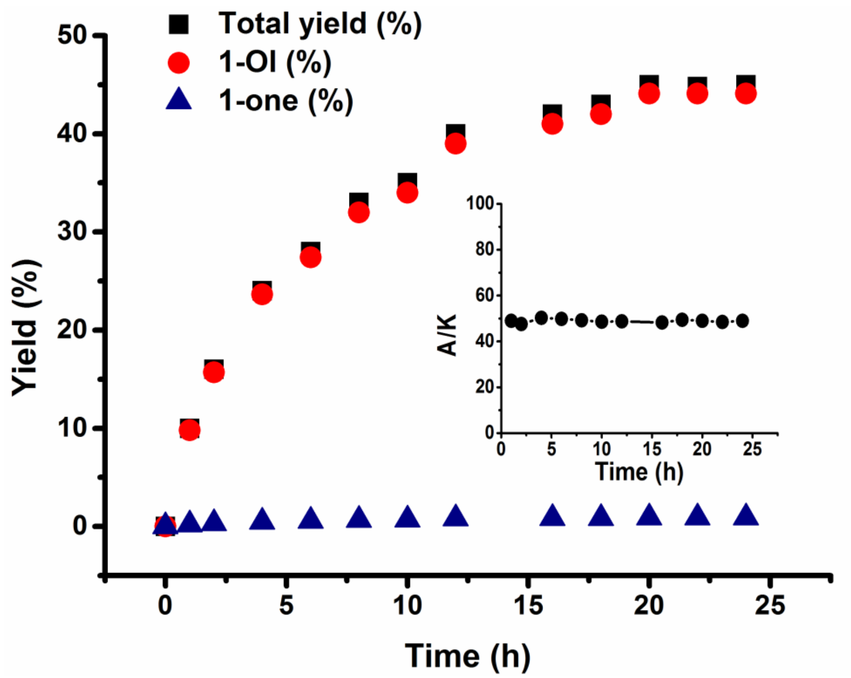

Figure S5. Accumulation of products in oxidation of cyclohexane by **1-Mont**/H_2O_2 with time at room temperature. (Inset: Change of A/K ratio with time)

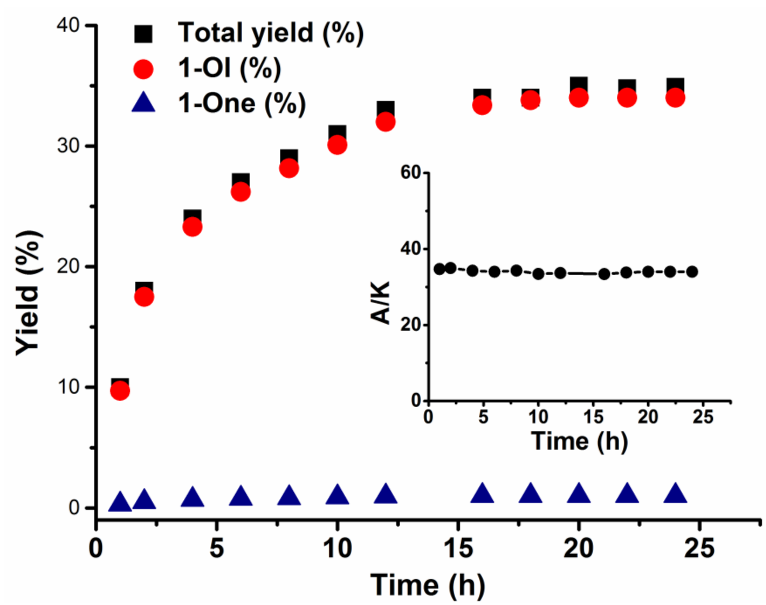

Figure S6. Accumulation of products in oxidation of cyclooctane by **1-Mont**/H_2O_2 with time at room temperature. (Inset: Change of A/K ratio with time)

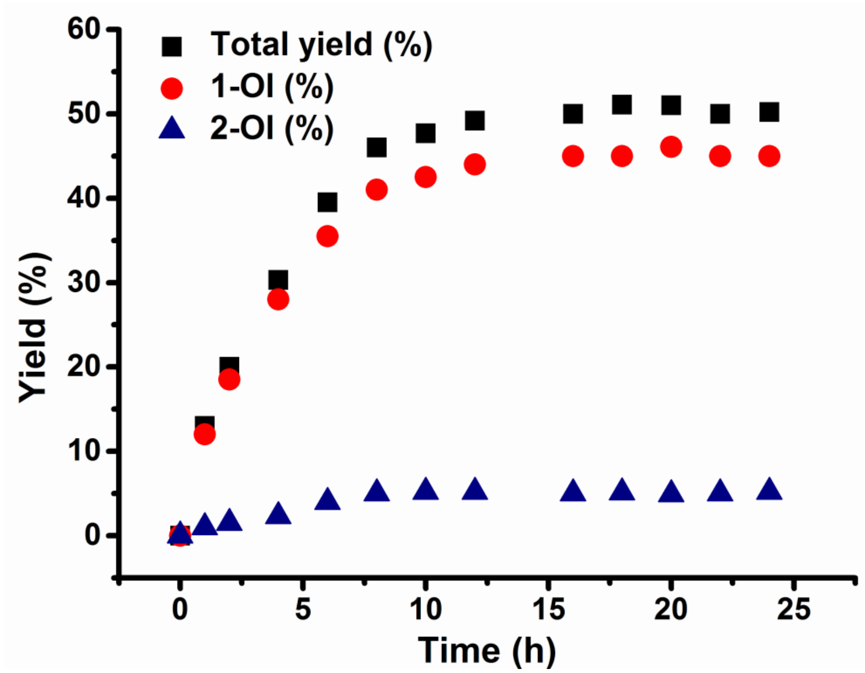

Figure S7. Accumulation of products in oxidation of adamantane by **1-Mont**/H_2O_2 with time at room temperature.

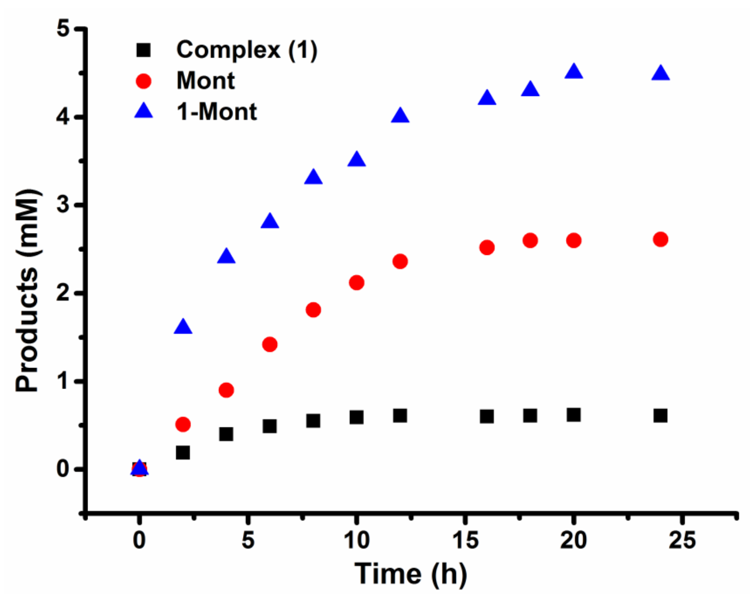

Figure S8. Time course accumulation of oxygenates during oxidation of cyclohexane catalyzed by **1**/H_2O_2, **Mont**/H_2O_2 and **1-Mont**/H_2O_2. The data have been analyzed by initial rate method and the rate constants are given in the main text.

Substrate Limiting Condition*

*Reaction condition: cyclohexane (2.5 mM), acetonitrile (2 mL), 20h, under argon at room temperature. Under Identical condition, reactions using 1 gave liitle or no product. Blank reaction without oxidant (H_2O_2) gave no product.

Table S1: Effect of H_2O_2 concentration on cyclohexane oxidation

Catalyst: **1-Mont** [60mg]
Solvent: Acetonitrile-[2ml],
Oxidant: H_2O_2 [Varied],
Argon atmosphere, Room temperature.
Substrate: Cyclohexane [2.5mM]

Entry	H_2O_2 (mM)	Yield[a]	Product Profile	
			Cyclohexanol	Cyclohexanone
1	2.5	2.6%	2.6%	0%
2	5.0	5.0%	5.0%	0%
3	10.0	5.3%	3.5%	1.5%
4	20.0	5.7%	4.0%	1.7%
5	40.0	6.1%	4.2%	1.9%

[a]Yield expressed with respect to substrate concentration

Table S2: Effect of **1-Mont** concentration on cyclohexane oxidation

Catalyst: **1-Mont** [Varied]
Solvent: Acetonitrile-[2ml],
Oxidant: H_2O_2[5mM],
Argon atmosphere, Room temperature.
Substrate: Cyclohexane [2.5mM]

Entry	1-Mont (mg)	Yield[a]	Product Profile	
			Cyclohexanol	Cyclohexanone
1	15	2.5%	2.5%	0%
2	30	2.8%	2.8%	0%
3	45	3.8%	3.8%	0%
4	60	5.0%	5.0%	0%
5	90	6.2%	6.2%	0%

[a]Yield expressed with respect to substrate concentration

Table S3: Effect of substrate concentration on cyclohexane oxidation

Catalyst: **1-Mont** [60mg]
Solvent: Acetonitrile-[2ml],
Oxidant: Hydrogen peroxide-[5mM],
Argon atmosphere, Room temperature.
Substrate: Cyclohexane [Varied]

Entry	Cyclohexane (mM)	Yield[a]	Product Profile	
			Cyclohexanol	Cyclohexanone
1	2.0	4.5%	4.5%	0%
2	2.5	5.0%	5.0%	0%
3	5.0	5.9%	5.9%	0%
4	7.5	6.8%	6.8%	0%
5	10.0	7.2%	7.2%	0%

[a]Yield expressed with respect to substrate concentration