

**Supporting Information
for
Trinuclear [Fe^{III}-Mg^{II}] compounds with aminopyridines as a precursor for supported
C=C bond hydrogenation catalysts at atmospheric pressure in plug-flow reactor**

Yana A. Tigai^a, Kseniya A. Koshenskova^a, Denis N. Nebykov^{b,*}, Anastasia V. Lagutina^b,
Vladimir M. Mokhov^b, Fedor M. Dolgushin^a, Lada S. Razvorotneva^a, Nikolay N. Efimov^a,
Konstantin A. Babeshkin^a, Natalia V. Gogoleva^a, Vladimir K. Imshennik^c, Sergey A.
Novichikhin^c, Igor L. Eremenko^a, and Irina A. Lutsenko^{a*}

^a*N.S. Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences, Leninsky Prospekt 31, 119991 GSP-1 Moscow, Russian Federation
Fax (495) 952 1279. E-mail: irinalu05@rambler.ru*

^b*Volgograd State Technical University, Prospekt Lenina 28, 400005 Volgograd, Russian Federation
E-mail: nervwho@gmail.com*

^c*Semenov Institute of Chemical Physics, Russian Academy of Sciences, Kosygina 4, 119991 Moscow, Russian Federation*

Table S1

Selected crystal data and parameters for structure refinement of the title compounds **1** and **2**

Compound	1	2
Formula	C ₃₅ H ₆₂ N ₂ O ₁₄ Fe ₂ Mg • 1.5CH ₃ CN	C ₃₅ H ₆₂ N ₂ O ₁₄ Fe ₂ Mg
Formula weight	932.45	870.87
Temperature (K)	100(2)	100(2)
Crystal system	monoclinic	monoclinic
Space group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> 2 ₁ / <i>c</i>
<i>a</i> (Å)	13.358(4)	11.9210(4)
<i>b</i> (Å)	28.564(8)	22.5802(8)
<i>c</i> (Å)	13.605(4)	17.5040(5)
<i>α</i> (deg)	90	90
<i>β</i> (deg)	101.078(10)	105.541(2)
<i>γ</i> (deg)	90	90
<i>V</i> (Å ³)	5094(3)	4539.4(3)
<i>Z</i>	4	4
<i>d</i> _{calc} (g·cm ⁻³)	1.216	1.274
<i>μ</i> (mm ⁻¹)	0.640	0.712
<i>F</i> (000)	1980	1848
2 θ range (deg)	4.2 to 56.0	3.6 to 60.0
Reflections collected	48153	120665
Independent reflections / <i>R</i> _{int}	12287 / 0.0466	13224 / 0.0553
Observed reflections <i>I</i> > 2 σ (<i>I</i>)	9723	11403
No of parameters	659	534
GooF on <i>F</i> ²	1.045	1.043
<i>R</i> ₁ (<i>I</i> > 2 σ (<i>I</i>))	0.0506	0.0317
<i>wR</i> ₂ (all data)	0.1187	0.0819
largest diff peak / hole (e ⁻ ·Å ⁻³)	0.700 / -0.543	0.536 / -0.539
CCDC number	2429782	2429783

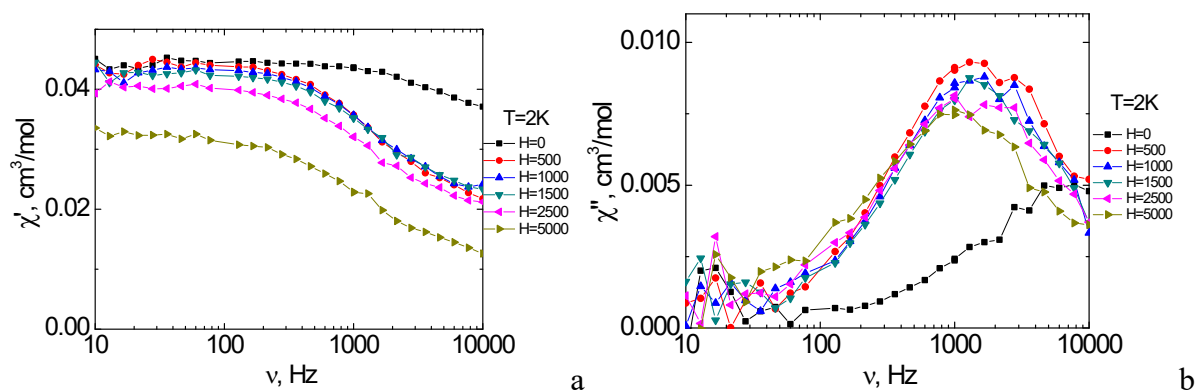


Fig. S1– Frequency dependences of the real (χ' , a) and imaginary (χ'' , b) parts of the dynamic magnetic susceptibility of complex1 in the range of magnetic fields from 0 up to 5000 Oe at temperature 2 K. The lines are guides for the eyes

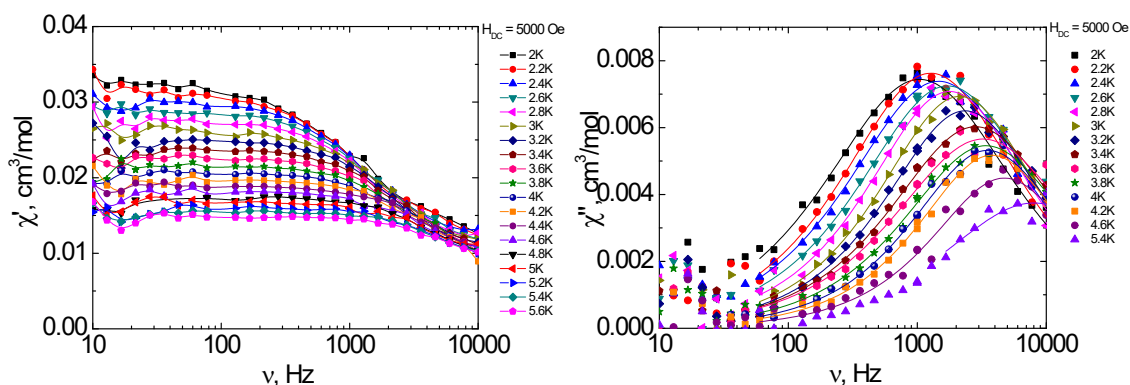


Fig. S2 – Frequency dependences of the real (χ' , a) and imaginary (χ'' , b) parts of the dynamic magnetic susceptibility of complex 1 in the temperature range of 2-5.4K at a magnetic field strength of 5000 Oe. The lines are a) guides for the eyes; b) the approximation of experimental data by the generalized Debye model.

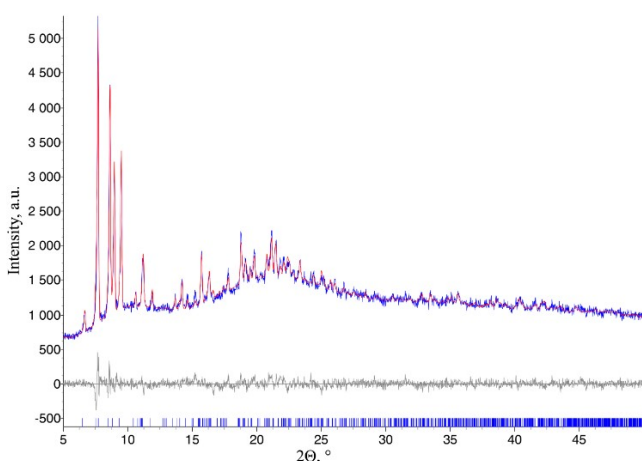


Fig. S3 – The experimental (blue line) and calculated (red line) powder patterns for 2 and their difference (grey curve). Ticks indicated calculated positions of the peaks.

