Supplementary Information

for

Extention and functionalization of an encapsulating macrobicyclic ligand using palladium-catalyzed Suzuki–Miyaura and Sonogashira reactions of the iron(II) dihalogenoclathrochelates with inherent halogen substituents

Irina N. Denisenko[a], Oleg A.Varzatskii[a], Roman A. Selin[a,e], Alexander S. Belov[b], Ekaterina G. Lebed[b], Anna V. Vologzhanina[b], Yan V. Zubavichus,[d] Yan Z. Voloshin[*,b,c]

[a] *Vernadskii Institute of General and Inorganic Chemistry NASU, 03142 Kiev, Ukraine*

[b] *Nesmeyanov Institute of Organoelement Compounds RAS, 119991 Moscow, Russia*

[c] *Kurnakov Institute of General and Inorganic Chemistry RAS, 119991 Moscow, Russia*

[d] *Kurchatov Complex for Synchrotron and Neutron Investigations, National Research Centre "Kurchatov Institute", 123182 Moscow, Russia*

[e] *PBMR Labs Ukraine, 02094 Kiev, Ukraine*

Table S1. Crystallographic data and refinement parameters for the obtained monoribbed-functionalized iron(II) clathrochelates.

Parametr	$FeBd_2((EtONaphth)_2Gm)(BF)_2 \cdot 3CH_2Cl_2$ (**1** · $3CH_2Cl_2$)	$FeBd_2((EtONaphth)_2Gm)(BF)_2$ (**1**)	$FeBd_2((Me_3Si)C{\equiv}CGmH)(BF)_2$ (**4**)
Empirical formula	$C_{57}H_{48}B_2Cl_6F_2FeN_6O_8$	$C_{54}H_{42}B_2F_2FeN_6O_8$	$C_{35}H_{30}B_2F_2FeN_6O_6Si$
Fw	1273.18	1018.40	774.21
T (K)	120	100	100
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	*P 2₁/c*	*C 2/c*	*P 2₁*
Z	4	4	2
a (Å)	17.9086(17)	20.219(4)	12.652(3)
b (Å)	15.6856(13)	14.037(3)	10.702(2)
c (Å)	31.456(3)	18.998(4)	13.227(3)
β (°)	139.855(2)	103.87(3)	90.42(3)
V (Å^3)	5696.9(9)	5234.8(19)	1790.9(6)
d_{calc} (g·cm^{-3})	1.484	1.292	1.436
μ (mm^{-1})	0.613	0.812	1.222
F(000)	2608	2104	796
$2\Omega_{max}$ (°)	59.2	76.8	76.9
Measured refl.	47833	26858	19586
Independent reflections (R_{int})	15863 (0.112)	5377 (0.079)	6974 (0.100)
Obs.refl./restraints/ parameters	7849 / 6 / 741	3229 / 0 / 279	5090 / 1 / 482
R [a] (%) [I > 2σ(I)]	0.0638	0.0881	0.0595
R_w [b] (%)	0.1174	0.2262	0.1578
GOF[c]	1.004	1.025	1.005
Residual electron density (e·Å^{-3}) (d_{min}/d_{max})	0.72 / –0.73	0.46 / –0.32	0.89 / –0.85
Flack			0.046(5)

[a] $R = \Sigma \, | \, |F_o| - |F_c| \, | / \Sigma \, |F_o|$. [b] $R_w = [\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma(w(F_o^2))]^{1/2}$. [c] $GOF = [\Sigma w(F_o^2 - F_c^2)^2/(N_{obs} - N_{param})]^{1/2}$