1

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

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

| Parameter | \(\text{FeBd}_2((\text{EtONaphth})_2\text{Gm})(\text{BF})_2\cdot3\text{CH}_2\text{Cl}_2\) (1) | \(\text{FeBd}_2((\text{EtONaphth})_2\text{Gm})(\text{BF})_2\) (1) | \(\text{FeBd}_2(\text{Me}_3\text{Si})\text{C≡CGmH})(\text{BF})_2\) (4) |
|-----------|---------------------------------|-----------------|-----------------|
| Crystallographic data | | | |
| Empirical formula | \(\text{C}_{37}\text{H}_{48}\text{B}_2\text{Cl}_2\text{F}_2\text{FeN}_6\text{O}_8\) | \(\text{C}_{34}\text{H}_{42}\text{B}_2\text{FeN}_6\text{O}_8\) | \(\text{C}_{35}\text{H}_{30}\text{B}_2\text{F}_2\text{FeN}_6\text{O}_6\text{Si}\) |
| \(\text{Fw}\) | 1273.18 | 1018.40 | 774.21 |
| \(\text{T (K)}\) | 120 | 100 | 100 |
| Crystal system | Monoclinic | Monoclinic | Monoclinic |
| Space group | \(P 2_1/c\) | \(C 2/c\) | \(P 2_1\) |
| \(Z\) | 4 | 4 | 2 |
| \(a (\text{Å})\) | 17.9086(17) | 20.219(4) | 12.652(3) |
| \(b (\text{Å})\) | 15.6856(13) | 14.037(3) | 10.702(2) |
| \(c (\text{Å})\) | 31.456(3) | 18.998(4) | 13.227(3) |
| \(\beta (^\circ)\) | 139.855(2) | 103.87(3) | 90.42(3) |
| \(V (\text{Å}^3)\) | 5696.9(9) | 5234.8(19) | 1790.9(6) |
| \(d_{\text{calc}} \text{ (g·cm}^{-3}\) | 1.484 | 1.292 | 1.436 |
| \(\mu \text{ (mm}^{-1}\) | 0.613 | 0.812 | 1.222 |
| \(F(000)\) | 2608 | 2104 | 796 |
| \(2\Omega_{\text{max}} (^\circ)\) | 59.2 | 76.8 | 76.9 |
| Measured refl. | 47833 | 26858 | 19586 |
| Independent reflections \((R_{\text{int}})\) | 15863 (0.112) | 5377 (0.079) | 6974 (0.100) |
| Obs. refl./restraints/parameters | 7849 / 6 / 741 | 3229 / 0 / 279 | 5090 / 1 / 482 |
| \(R\) \(^a\) \([I > 2\sigma(I)]\) | 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 \((\text{e·Å}^{-3}\) | 0.72 / –0.73 | 0.46 / –0.32 | 0.89 / –0.85 |
| \(d_{\text{min}}/d_{\text{max}}\) | | | |
| 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_{\text{obs}} - N_{\text{param}})]^{1/2}\).