Supplementary Material (ESI) for Chemical Communications

Crystal data for all adducts were collected either at 293 K (**1·adipic(4)**, **1·pimelic(5)**, **1·suberic(6)**, **1·sebacic(8)**) or at 273 K (**1·azelaic(7)**) on a Brucker APEX II diffractometer [monochromator graphite, MoKα radiation (λ = 0.71073 Å)]. Crystals suitable for diffraction experiments were difficult to grow, in most cases polycrystalline powders were obtained with only few poorly formed single crystals. For all compounds, Z is referred to the number of macrocycles in the unit cell.

1·adipic(4): $\{[Fe(\eta^5\text{-}C_5H_4\text{-}C_5H_4N)_2]\cdot[HOOC(CH_2)_4COOH]\}_2$, M = 972.68, triclinic, P-1, a = 11.276 (2), b = 14.816(3), c = 28.600(6) Å, α = 89.201(4), β = 87.275(4), γ = 68.551(3) °, V = 4442(2) Å^3, Z = 4, μ = 0.716, 15394 independent reflections (31703 measured), wR_2 (all data) = 0.3563, R_1 (I >2σ(I)) = 0.1189.

1·pimelic(5): $\{[Fe(\eta^5\text{-}C_5H_4\text{-}C_5H_4N)_2]\cdot[HOOC(CH_2)_5COOH]\}_2$, M = 2001.46, P-1, a = 9.396 (2), b = 10.667(3), c = 24.172(2) Å, α = 78.03(5), β = 88.93(2), γ = 81.25(4) °, V = 2342.2(8) Å^3, Z = 1, μ = 0.681, 8019 independent reflections (16818 measured), wR_2 (all data) = 0.1990, R_1 (I >2σ(I)) = 0.0645.

1·suberic(6): $\{[Fe(\eta^5\text{-}C_5H_4\text{-}C_5H_4N)_2]\cdot[HOOC(CH_2)_6COOH]\}_2$, M = 1028.78, monoclinic, $P2_1/c$, a = 11.107(9), b = 31.467(18), c = 14.846(12) Å, β = 110.33(8) °, V = 4866(6) Å^3, Z = 4, μ = 0.658, 7134 independent reflections (15533 measured), wR_2 (all data) = 0.4224, R_1 (I >2σ(I)) = 0.1271 (Only 83% of data collection completed, because of crystal decay).

1·azelaic(7): $\{[Fe(\eta^5\text{-}C_5H_4\text{-}C_5H_4N)_2]\cdot[HOOC(CH_2)_7COOH]\}_2$, M = 1056.83, triclinic, P-1, a = 9.8845(5), b = 10.7413(6), c = 13.4321(7) Å, α = 76.177(1), β = 78.844(1), γ = 68.146(1)°, V = 1276.6(1) Å^3, Z = 1, μ = 0.629, 5782 independent reflections (11137 measured), wR_2 (all data) = 0.1046, R_1 (I >2σ(I)) = 0.0390.

1·sebacic(8): $\{[Fe(\eta^5\text{-}C_5H_4\text{-}C_5H_4N)_2]\cdot[HOOC(CH_2)_8COOH]\}_2$, M = 1084.88, triclinic, P-1, a = 11.028(2), b = 13.747(3), c = 18.765(4) Å, α = 96.076(3), β = 102.689(3), γ = 105.048(3)°, V = 2639.6(9) Å^3, Z = 2, μ = 0.610, 5277 independent reflections (12282 measured), wR_2 (all data) = 0.2152, R_1 (I >2σ(I)) = 0.0694.

SHELX97[1a] and SCHAKAL99[1b] were used for structure solution and graphical representations. CCDC 614138–614141.

1 (a) G. M. Sheldrick, SHELXL97: Program for Crystal Structure Determination, University of Göttingen, Germany, 1997; (b) E. Keller, SCHAKAL99: Graphical Representation of Molecular Models, University of Freiburg, Germany, 1999; (c) W. Kraus and G. Nolze, PowderCell 2.2 (BAM Berlin) © subgroups derived by Ulrich Müller (Gh Kassel)].