

Supplementary Information

to

A (bpy)₂Ru-coordinated dehydro[12]annulene with exotopically fused diimine binding sites

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Analytical data for ruthenium complexes 1, 11 and 12:

Complex 1:

¹H-NMR (CD₃CN, 500 MHz): δ = 9.57 (d, J = 8.1 Hz, 4 H, γ CH), 8.55 (d, J = 8.2 Hz, 4 H, δ bpy), 8.52 (d, J = 8.2 Hz, 4 H, δ bpy), 8.37 (s, 4 H, phenazine CH), 8.19 (d, J = 5.5 Hz, 4 H, α CH), 8.11 (m, 4 H, γ bpy), 8.03 (m, 4 H, γ bpy), 7.89 (dd, J = 8.1, 5.5 Hz, 4 H, β CH), 7.84 (m, 4 H, α bpy), 7.72 (m, 4 H, α bpy), 7.46 (m, 4 H, β bpy), 7.27 (m, 4 H, β bpy)

MALDI-TOF, m/z (%): 1919 (100) [M^+ - 1 PF₆], 1773 (30) [M^+ - 2 PF₆]

Elemental analysis: calcd. (Ru₂C₈₄H₄₈N₁₆(PF₆)₄• 8 H₂O): C 45.6, H 2.8, N 10.1; found C 45.3, H 2.9, N 8.7

Complex 11:

¹H-NMR (DMSO-d₆, 500 MHz): δ = 9.60 (d, J = 8.2 Hz, 2 H, γ CH), 8.86 (d, J = 8.2 Hz, 2 H, δ bpy), 8.83 (d, J = 8.2 Hz, 2 H, δ bpy), 8.59 (s, 2 H, phenazine CH), 8.22 (m, 4 H, α CH, γ bpy), 8.13 (m, 2 H, γ bpy), 8.02 (dd, J = 8.2, 5.5 Hz, 2 H, β CH), 7.81 (m, 2 H, α bpy), 7.76 (m, 2 H, α bpy), 7.59 (m, 2 H, β bpy), 7.38 (m, 2 H, β bpy), 1.18 (m, 42 H, *i*-Pr)

FAB-MS, m/z (%): 1201 (4) [M^+ - 1 PF₆], 1056 (6) [M^+ - 2 PF₆]

Elemental analysis: calcd. (RuC₆₀H₆₆N₈Si₂(PF₆)₂•H₂O): C 52.8, H 4.9 N 8.2; found C 53.1, H 5.0, N 8.0

Complex 12:

$^1\text{H-NMR}$ (CD_3CN , 500 MHz): δ = 9.60-9.58 (m, 4 H, γ CH), 8.69 (2 s, 2 H, phenazine CH), 8.66 (2 s, 2 H, phenazine CH), 8.60 (d, J = 8.2 Hz, 4 H, δ bpy), 8.56 (d, J = 8.2 Hz, 4 H, δ bpy), 8.19 (dd, J = 4.3, 1.0 Hz, 4 H, α CH), 8.11 (m, 4 H, γ bpy), 8.02 (m, 4 H, γ bpy), 7.91-7.85 (m, 4 H, β CH), 7.84 (m, 4 H, α bpy), 7.72 (m, 4 H, α bpy), 7.46 (m, 4 H, β bpy), 7.27 (m, 4 H, β bpy), 1.26 (m, 42 H, *i*-Pr)

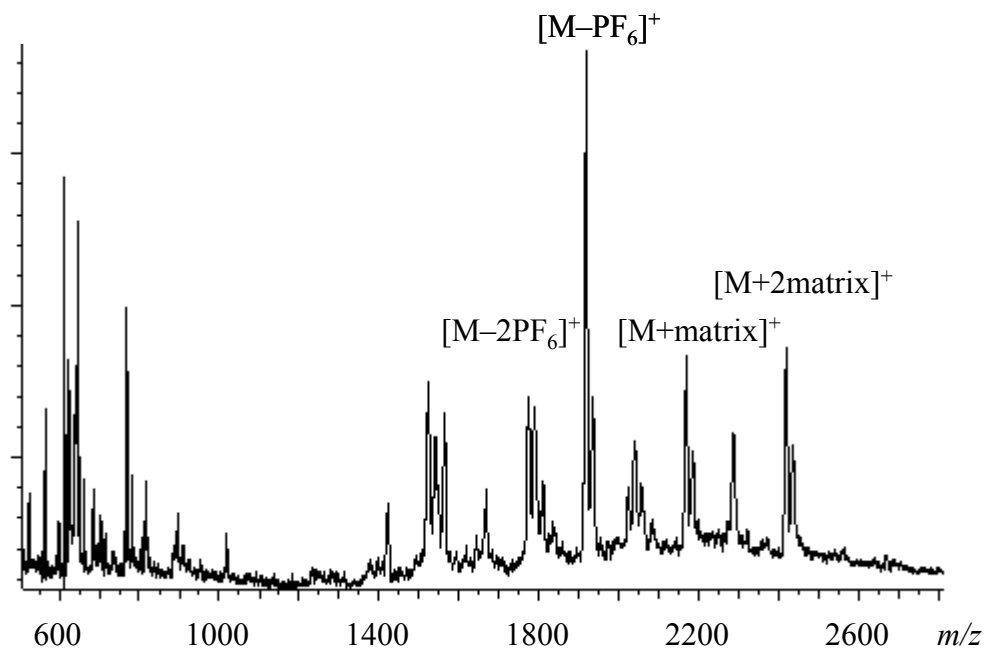
MALDI-TOF , m/z (%): 2233 (100) $[\text{M}^+ - 1 \text{PF}_6]$, 2089 (20) $[\text{M}^+ - 2 \text{PF}_6]$

Elemental analysis: calcd. ($\text{Ru}_2\text{C}_{102}\text{H}_{90}\text{N}_{16}\text{Si}_2(\text{PF}_6)_4 \bullet 2 \text{H}_2\text{O}$): C 50.7, H 3.8, N 9.3; found C 51.0, H 3.7, N 8.7

MALDI-TOF mass spectrum of **1**: Calcd. mass for $\text{Ru}_2\text{C}_{84}\text{H}_{48}\text{N}_{16}(\text{PF}_6)_4$: 2063 g M^{-1} ;

Found: 1919 (100) $[\text{M}^+ - 1 \text{PF}_6]$, 1773 (30) $[\text{M}^+ - 2 \text{PF}_6]$.

2-[(2*E*)-3-(4-*tert*-butylphenyl)-2-methylprop-2-enylidene] malononitrileⁱ was used as matrix.



ⁱ T. Brown, N. L. Clipston, N. Simjee, H. Luftmann, H. Hungerbuehler, T. Drewello, *Int. J. Mass Spectr.*, **2001**, 210/211, 249-263.