

## Synthesis, characterization and crystal structure of

$[\text{Ru}(\text{tppz})(4,4'-(\text{CH}_3)_2\text{bpy})\text{Cl}](\text{PF}_6)$ , (tppz = 2,3,5,6-tetrakis(2-pyridyl)pyrazine)

Tondreau, Valeria

Leiva, Ana Maria

Loeb, Barbara

Boys, Daphne

Stultz, Laura K.

Meyer, Thomas J.

The synthesis and characterization of the complex  $[\text{Ru}(\text{tppz})(4,4'-(\text{CH}_3)_2\text{bpy})\text{Cl}]^+$ , where tppz = 2,3,5,6-tetrakis(2-pyridyl)pyrazine, is reported. The ion was obtained in a one pot synthesis by reduction of  $\text{Ru}(4,4'-(\text{CH}_3)_2\text{bpy})\text{Cl}_4$  with triethylamine in the presence of tppz, and isolated as the hexafluorophosphate salt. The structure of  $[\text{Ru}(\text{tppz})(4,4'-(\text{CH}_3)_2\text{bpy})\text{Cl}](\text{PF}_6)$ , **1**, was established by X-ray diffraction. The ruthenium atom is in a highly distorted octahedral environment with the 4,4'-(CH<sub>3</sub>)<sub>2</sub>bpy nitrogens, the pyrazine central nitrogen of tppz, and chlorine defining the best mean equatorial plane. The axial positions are occupied by the nitrogens of the coordinated pyridyl rings of tppz. The Ru - N(tppz) bond to the central ring is short [1.962(9) Å], while the Ru - N(4,4'-(CH<sub>3</sub>)<sub>2</sub>bpy) bond trans to it is lengthened towards a single bond distance [2.096(10) Å]. This enhances the distortion in coordination of the octahedron, mainly produced by the bite angle of tppz. The distortions in **1**