Electronic Supplementary Information for Dalton Transactions

Electronic supplementary information

Pseudo-base formation in the attempted synthesis of a conjugatively coupled bis(nitrosylruthenium) complex and spectroelectrochemistry of bipyrimidine-bridged dinuclear Ru(terpy)X precursor compounds (X = Cl, NO_2)

Priti Singh, Monika Sieger, Jan Fiedler, Cheng-Yong Su and Wolfgang Kaim*

Table S1. Structure parameters (bond lengths in Å, bond angles in deg) of complex {(μ-bpym-(4-OH))[Ru(NO)(terpy)]$_2$}$(PF_6)_5$·2.5H_2O.

Ru(1)- N(11)	1.784(5)
Ru(1)-N(9)	1.993(5)
Ru(1)-N(4)	2.066(5)
Ru(1)-N(10)	2.085(6)
Ru(1)-N(8)	2.088(6)
Ru(1)-N(3)	2.121(5)
Ru(2)-N(12)	1.796(5)
Ru(2)-N(6)	1.990(5)
Ru(2)-N(2)	2.068(5)
Ru(2)-N(7)	2.069(6)
Ru(2)-N(5)	2.092(6)
Ru(2)-N(1)	2.133(5)
N(1)-C(4)	1.331(8)
N(1)-C(1)	1.337(8)
N(2)-C(5)	1.315(8)
N(2)-C(8)	1.471(8)
N(3)-C(3)	1.334(8)
N(3)-C(4)	1.338(8)
N(4)-C(5)	1.343(8)
N(4)-C(6)	1.410(8)
N(5)-C(9)	1.319(9)
N(11)-O(1)	1.121(7)
N(12)-O(2)	1.101(6)

C(1)-C(2)	1.373(10)
C(2)-C(3)	1.388(10)
C(4)-C(5)	1.452(9)
C(6)-C(7)	1.293(9)
C(7)-C(8)	1.474(9)
C(8)-O(3)	1.407(9)

O(1)-N(11)-Ru(1)	174.1(5)
O(2)-N(12)-Ru(2)	172.3(5)
O(3)-C(8)-N(2)	109.1(6)
N(11)-Ru(1)-N(9)	95.5(2)
N(11)-Ru(1)-N(4)	169.8(2)
N(9)-Ru(1)-N(4)	91.2(2)
N(11)-Ru(1)-N(10)	91.6(2)
N(9)-Ru(1)-N(10)	79.7(2)
N(4)-Ru(1)-N(10)	81.9(2)
N(11)-Ru(1)-N(8)	96.0(2)
N(9)-Ru(1)-N(8)	80.0(2)
N(4)-Ru(1)-N(8)	92.7(2)
N(10)-Ru(1)-N(8)	158.9(2)
N(11)-Ru(1)-N(3)	94.9(2)
N(9)-Ru(1)-N(3)	169.6(2)
N(4)-Ru(1)-N(3)	78.5(2)
N(10)-Ru(1)-N(3)	100.2(2)
N(8)-Ru(1)-N(3)	98.7(2)

N(12)-Ru(2)-N(6)	98.0(2)
N(12)-Ru(2)-N(2)	171.1(2)
N(6)-Ru(2)-N(2)	89.9(2)
N(12)-Ru(2)-N(7)	93.9(2)
N(6)-Ru(2)-N(7)	79.6(2)
N(2)-Ru(2)-N(7)	91.3(2)
N(12)-Ru(2)-N(5)	91.8(2)
N(6)-Ru(2)-N(5)	79.9(2)
N(2)-Ru(2)-N(5)	85.7(2)
N(7)-Ru(2)-N(5)	159.3(2)
N(12)-Ru(2)-N(1)	93.3(2)
N(6)-Ru(2)-N(1)	168.7(2)
N(7)-Ru(2)-N(1)	100.6(2)
N(5)-Ru(2)-N(1)	98.9(2)
N(2)-Ru(2)-N(1)	78.8 (2)