Electronic Supplementary Information for Dalton Transactions

Supplementary Information

Valence structures of the diastereomeric complexes *meso*- and *rac*-$[Ru_2(acac)_4(\mu\text{-}Q)]^n$ (n = 2–,–,0,+, 2+) with the multiply quinonoid bridging ligand Q = 1,2,4,5-tetraimino-3,6-diketocyclohexane

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Table S1. Crystal data for **1**.2H_2O

	1·2H_2O
molecular formula	C_{26} H_{36} N_4 O_{12} Ru_2
fw	798.73
crystal system	triclinic
space group	*P*–1
a (Å)	7.762(3)
b (Å)	14.41(2)
c (Å)	14.4522(13)
α(deg)	77.566(3)
β(deg)	85.492(8)
γ(deg)	89.57(3)
V(Å^3)	1574(2)
Z	2
μ(mm^{-1})	1.025
T (K)	150(2)
D_{calcd} (g cm^{-3})	1.677
F (000)	800
θ range(deg)	3.02 to30.00
Data/Restraints/Parameters	8970 / 353 / 405
R1, wR2 *[*I > 2σ(I)*]*	0.2411, 0.4924
R1, wR2(all data)	0.3239, 0.5299
GOF	1.484
largest diff. peak/hole, (e Å^{-3})	14.325, –2.656

Table S2. Selected bond distances (Å) and angles (^{o}) for **1**.2H_2O

Bond Lengths		Bond Angles	
Ru(1)-N(1)	1.918(15)	N(1)-Ru(1)-N(2)	82.7(7)
Ru(1)-N(2)	1.876(17)	N(3)-Ru(2)-N(4)	78.5(7)
Ru(2)-N(3)	1.973(15)		
Ru(2)-N(4)	1.876(15)		
N(1)-C(11)	1.31(3)		
N(2)-C(12)	1.30(2)		
C(12)-C(13)	1.44(3)		
C(13)-O(5)	1.25(2)		
N(3)-C(25)	1.28(2)		
N(4)-C(24)	1.29(3)		
C(24)-C(25)	1.41(3)		
C(26)-O(10)	1.22(2)		

Fig. S1. Mass spectra of (a) **1** and (b) **2** in CH_2Cl_2. Ionization probe: ESI. Analyser: Quadruple and time of flight. Detector: Micro channel plate detector (MCP)

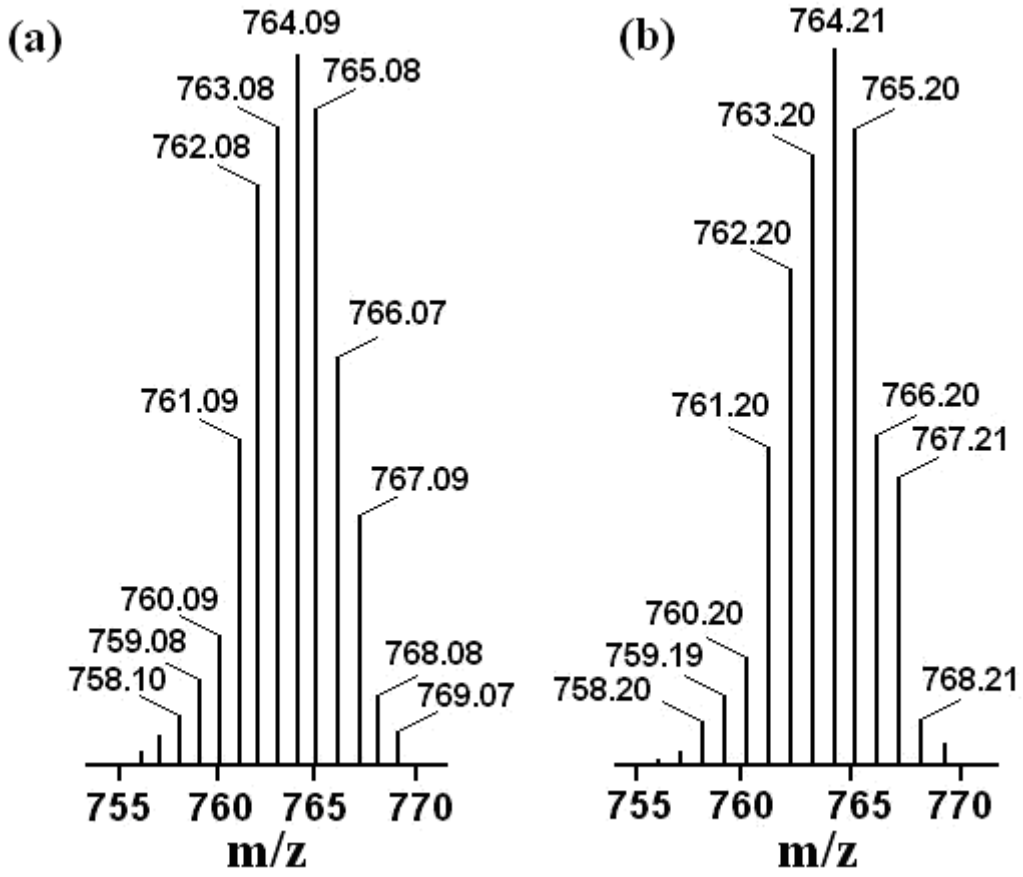

Fig. S2. IR spectra of (a) **1** and (b) **2** in KBr disk.

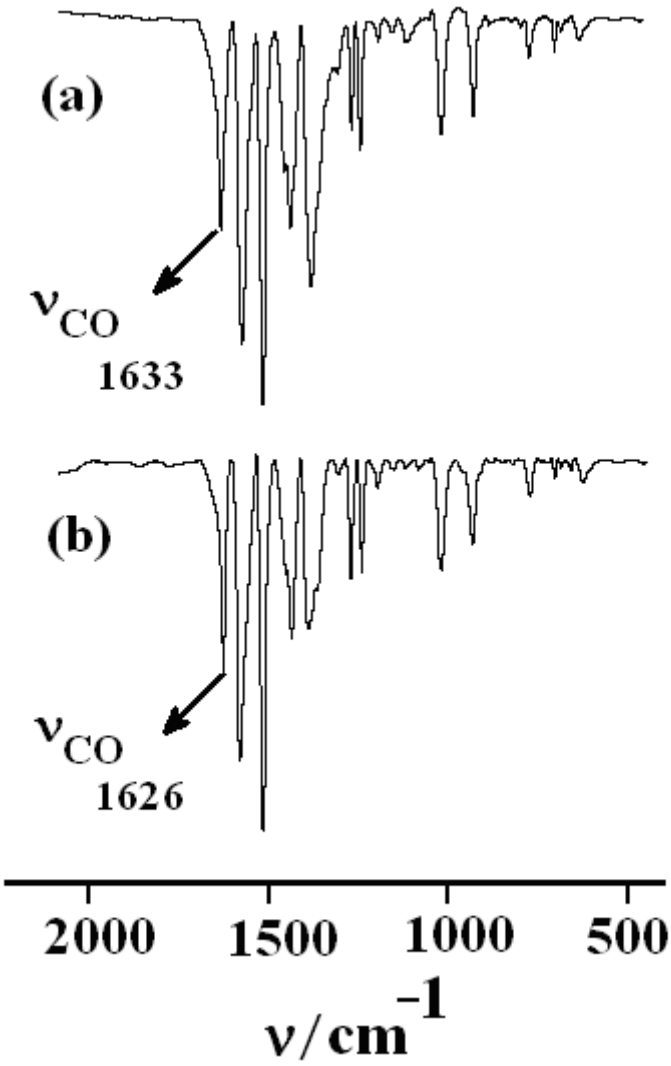

Fig. S3. ^{1}H NMR spectra of (a) **1** and (b) **2** in $CDCl_3$.