Sensitised near-infrared luminescence from lanthanide(III) centres using Re(I) and Pt(II) diimine complexes as energy donors in d-f dinuclear complexes based on 2,3-bis(2-pyridyl)pyrazine

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Supporting information: Crystal structure of $[Re(CO)_3Cl(dpq)][Gd(hfac)_3(H_2O)_2]\bullet C_6H_6$

Table S1. Crystal data, data collection and refinement details for $[Re(CO)_3Cl(dpq)][Gd(hfac)_3(H_2O)_2]\bullet C_6H_6$

Complex	$[Re(CO)_3Cl(dpq)]$ $[Gd(hfac)_3(H_2O)_2]\bullet C_6H_6$
Formula	$C_{42}H_{21}ClF_{18}GdN_4O_{11}Re$
Formula weight	1478.53
T (K)	173(2)
Crystal system, space group	Triclinic, P–1
a (Å)	9.525(2)
b (Å)	13.034(3)
c (Å)	23.796(6)
α (°)	105.83(3)
β (°)	90.746(19)
γ (°)	108.622(17)
V (Å^3)	2677.0(11)
Z	2
D_{calc}(Mg/m^3)	1.834
μ (mm^{-1})	3.656
Reflections (total, independent, R_{int})	22934, 9403, 0.0437
Data / restraints / parameters	9403, 37, 618
Final $R1$, $wR2$ indices[b]	0.0649, 0.1907

Table S2. Selected bond distances (Å) and angles (˚) for the structure of $[Re(CO)_3Cl(dpq)][Gd(hfac)_3(H_2O)_2]\bullet C_6H_6$

Gd(1)-O(115)	2.335(10)	Re(1)-C(41)	1.914(11)
Gd(1)-O(125)	2.323(12)	Re(1)-C(51)	1.916(11)
Gd(1)-O(111)	2.356(10)	Re(1)-C(61)	1.912(12)
Gd(1)-O(135)	2.393(10)	Re(1)-N(11)	2.164(8)
Gd(1)-O(2)	2.385(8)	Re(1)-N(21)	2.243(8)
Gd(1)-O(121)	2.377(11)	Re(1)-Cl(5)	2.469(3)
Gd(1)-O(131)	2.400(8)		
Gd(1)-O(1)	2.432(12)		
C(41)-Re(1)-C(51)	90.3(5)	C(61)-Re(1)-N(21)	104.5(4)
C(41)-Re(1)-C(61)	85.3(4)	N(11)-Re(1)-N(21)	74.6(3)
C(51)-Re(1)-C(61)	89.6(4)	C(41)-Re(1)-Cl(5)	92.2(3)
C(41)-Re(1)-N(11)	95.5(4)	C(51)-Re(1)-Cl(5)	177.1(3)
C(51)-Re(1)-N(11)	92.0(4)	C(61)-Re(1)-Cl(5)	92.2(3)
C(61)-Re(1)-N(11)	178.3(4)	N(11)-Re(1)-Cl(5)	86.2(2)
C(41)-Re(1)-N(21)	168.8(4)	N(21)-Re(1)-Cl(5)	82.0(2)
C(51)-Re(1)-N(21)	95.4(4)		

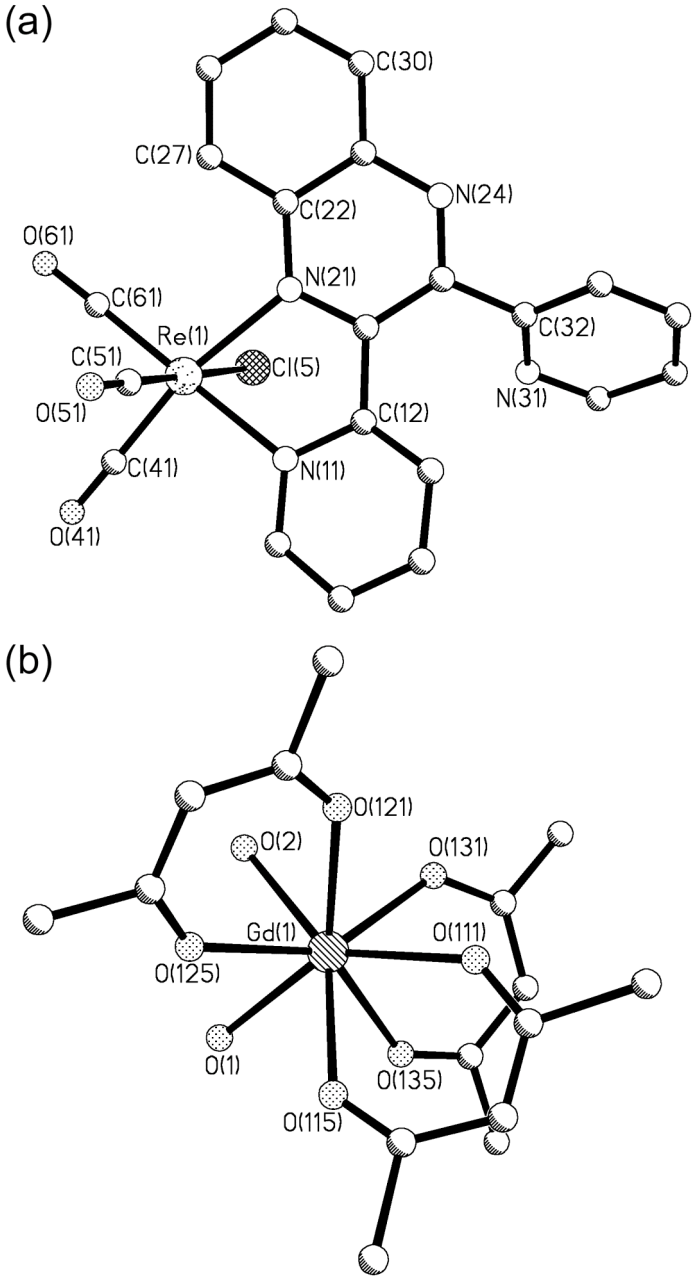

Fig. S1: Molecular structures of (a) the $[Re(CO)_3Cl(dpq)]$ complex unit and (b) the $[Gd(hfac)_3(H_2O)_2]$ complex unit, from crystals of $[Re(CO)_3Cl(dpq)][Gd(hfac)_3(H_2O)_2]\bullet C_6H_6$

In the $[Re(CO)_3Cl(dpq)]$ complex unit the coordinated and free pyridyl rings are twisted from the plane of the coordinated quinoxaline unit by 24˚ and 45˚ respectively. In the $[Gd(hfac)_3(H_2O)_2]$ unit the Gd(III) centre has an 8-coordinate square antiprismatic geometry, with the oxygen atoms of the two water ligands [O(1) and O(2)] and one of the hfac ligands [O(131) and O(135)] forming one approximate square plane, and the oxygen atoms of the remaining two hfac ligands [O(111), O(115), O(121), O(125)] forming the other.