

SUPPORTING INFORMATION

Syntheses, crystal structures, and magnetic properties of cyanide-bridged complexes *trans*-Ru^{II}(dppe)₂(CN)₂(Fe^{III}X₃)₂ (X = Cl and Br)

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Table S1. Crystallographic Data and Details of Structure Determination for Complexes **1-3**

Complex	1 ·2C ₃ H ₈ O	2	3
Chemical formula	C _{59.73} H ₆₄ Cl _{0.27} N _{1.74} O ₂ P ₄ Ru	C _{53.71} H ₄₈ Cl _{6.30} Fe ₂ N _{1.71} P ₄ Ru	C ₅₄ H ₄₈ Br ₆ Fe ₂ N ₂ P ₄ Ru
Formula weight	1072.58	1277.07	1541.05
Colour and Habit	Yellow prism	Red prism	Brown prism
Crystal Size / mm	0.367×0.336×0.133	0.281×0.162×0.127	0.452×0.236×0.128
T / K	123	123	123
Crystal system	Orthorhombic	Monoclinic	Triclinic
Space group	<i>Pccn</i>	<i>P2₁/n</i>	<i>P-1</i>
<i>a</i> / Å	22.513(9)	10.550(3)	11.495(4)
<i>b</i> / Å	13.334(5)	17.457(4)	11.698(4)
<i>c</i> / Å	17.261(7)	14.548(4)	12.087(5)
α / deg	90.00	90.00	109.785(3)
β / deg	90.00	97.216(4)	103.350(3)
γ / deg	90.00	90.00	103.136(3)
<i>V</i> / Å ³	5182(4)	2658.0(12)	1402.9(9)
Z	4	2	1
ρ_{calcd} (g/cm ³)	1.375	1.596	1.824
λ (Mo K _α , Å)	0.71073	0.71073	0.71073
μ (Mo K _α , mm ⁻¹)	0.485	1.295	5.200
Completeness	97.6%	99.7%	97.0%
<i>F</i> (000)	2236	1290	752
<i>h, k, l</i> , range	-29≤ <i>h</i> ≤27, -17≤ <i>k</i> ≤17, -22≤ <i>l</i> ≤21	-13≤ <i>h</i> ≤13, -22≤ <i>k</i> ≤21, -17≤ <i>l</i> ≤18	-14≤ <i>h</i> ≤14, -15≤ <i>k</i> ≤15, -15≤ <i>l</i> ≤15
θ range / deg	2.53-27.41	2.54-27.53	2.84-27.47
Reflections measured	5774	6116	6224
<i>R</i> _{int}	0.0460	0.0392	0.0337
Params/restraints/Data(obs.)	325/18/5582	323/36/5225	313/0/5845
GOF	1.007	1.011	1.008
R_1 , ωR_2 ($I > 2\sigma(I)$)	0.0363, 0.0952	0.0380, 0.1045	0.0358, 0.0971
R_1 , ωR_2 (all data)	0.0375, 0.0963	0.0435, 0.1074	0.0376, 0.0990

Table S2. Selected Bond Lengths (\AA) and Bond Angles (deg) for Complexes **1-3**

Complex	1	2	3
Ru-C	2.084(9)	2.007(17)	2.012(3)
Ru-Cl	2.45(2)	2.33(3)	
Ru1-P1	2.3896(8)	2.3954(9)	2.4001(9)
Ru1-P2	2.3622(7)	2.4135(9)	2.3924(9)
C≡N	1.143(11)	1.161(18)	1.141(3)
C-Ru-C	180.0(1)	180.0(2)	180.0(1)
N≡C-Ru	175.7(9)	177.3(14)	176.7(2)
C≡N-Fe		165.2(9)	165.2(2)
Fe-N1		1.957(5)	1.966(2)
Fe-X1		2.1569(12)	2.3161(9)
Fe-X2		2.1830(11)	2.3288(7)
Fe-X3		2.1745(11)	2.3194(10)
Fe…Ru		5.075	5.068
Fe…Fe(intramolecular)		10.150	10.137
Fe…Fe(intermolecular)		7.439	6.822
Ru…Fe(-NC-)		5.124	5.119
Fe…Fe(-NC-Ru-CN-)		10.248	10.238

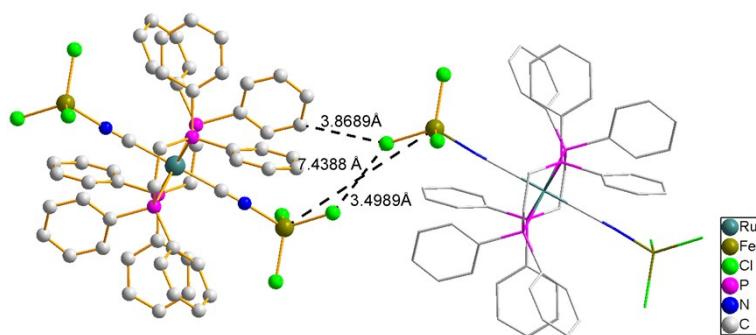


Figure S1 Packing structure of complex **2**.

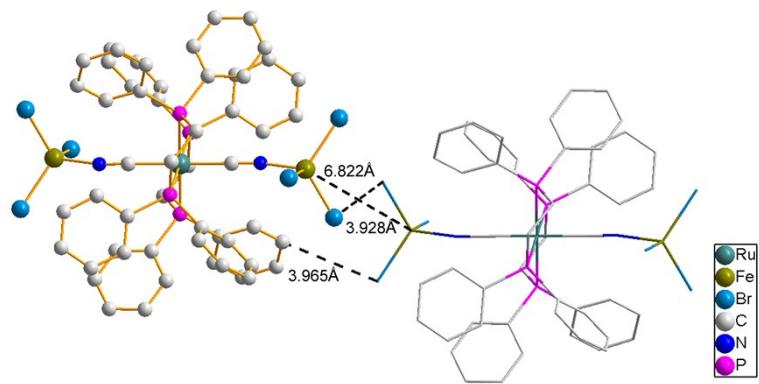


Figure S2 Packing structure of complex 3.

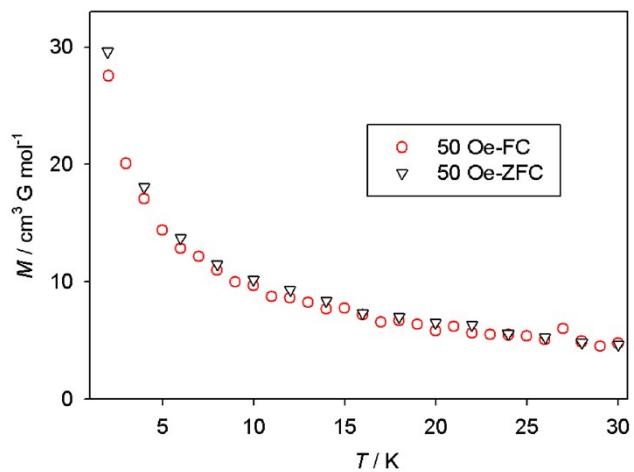


Figure S3 ZFC and FC magnetization of **2** at 50 Oe warming from 2 K to 30 K

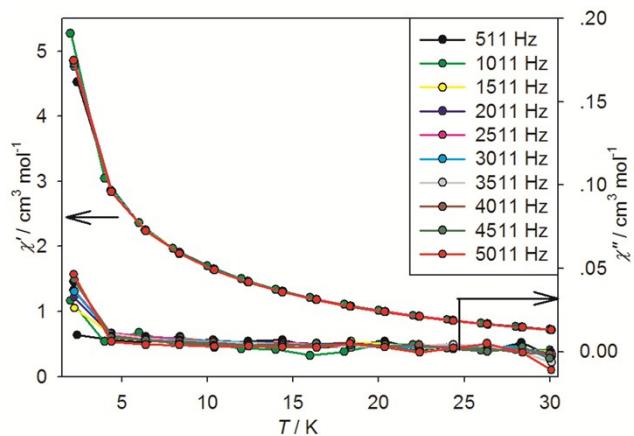


Figure S4. Temperature dependence of the in-phase and out-of-phase ac susceptibility for **2** in zero dc and 3 Oe ac applied field

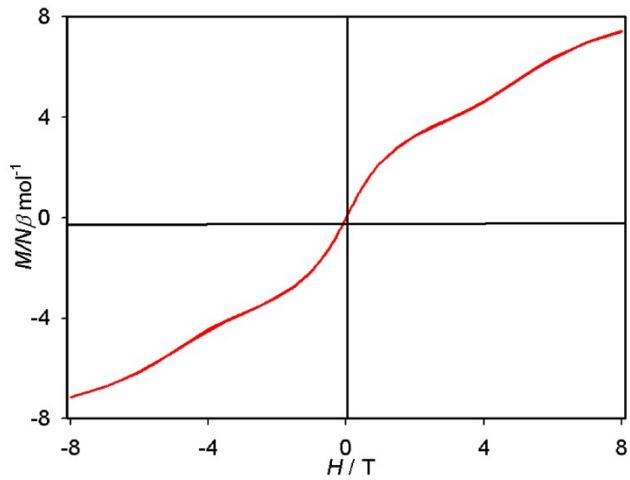


Figure S5. Plot of $M/N\beta$ vs H for the sample **2** at 2 K.

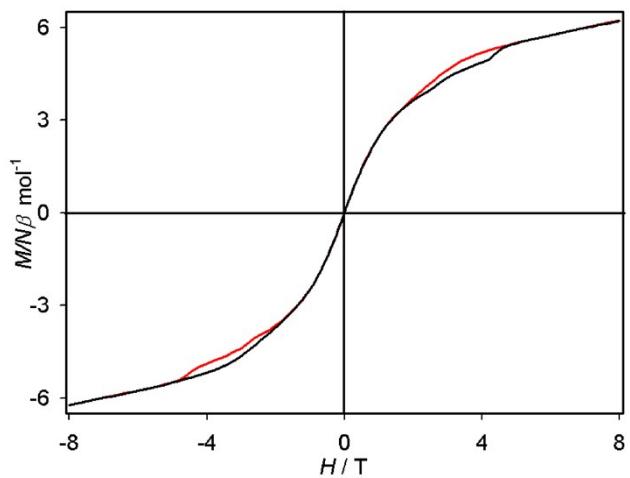


Figure S6 Plot of $M/N\beta$ vs H for the sample **3** at 2 K.

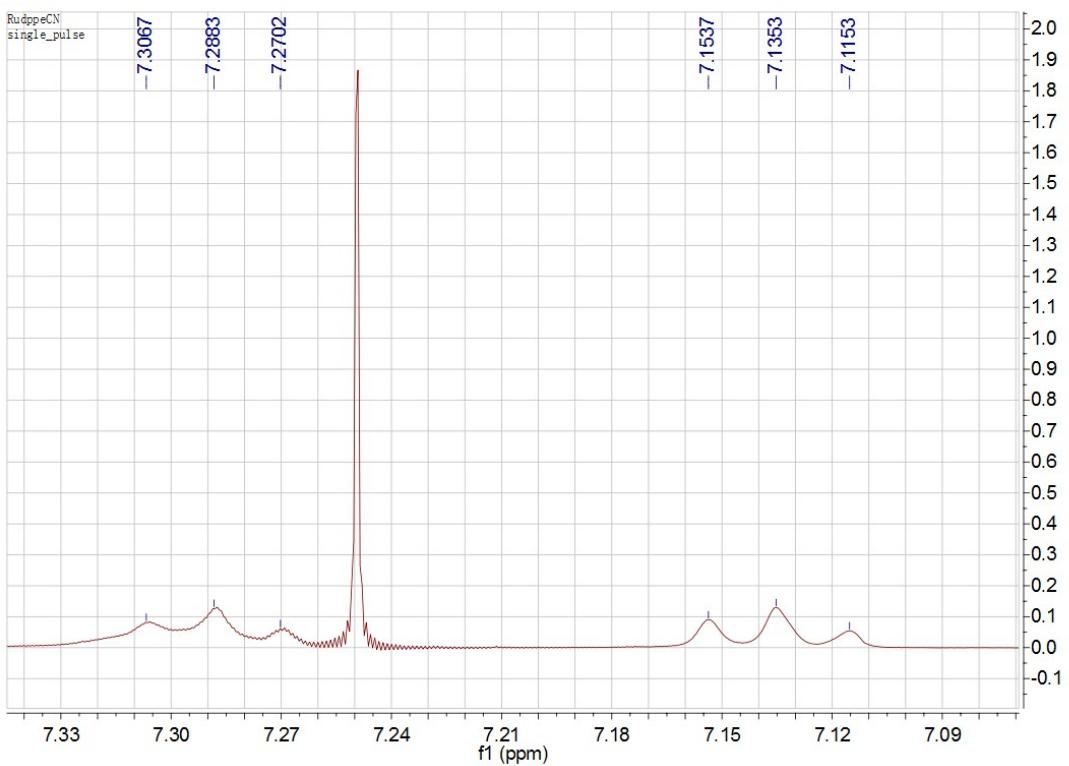


Figure S7 ^1H NMR of complex **1** in CDCl_3

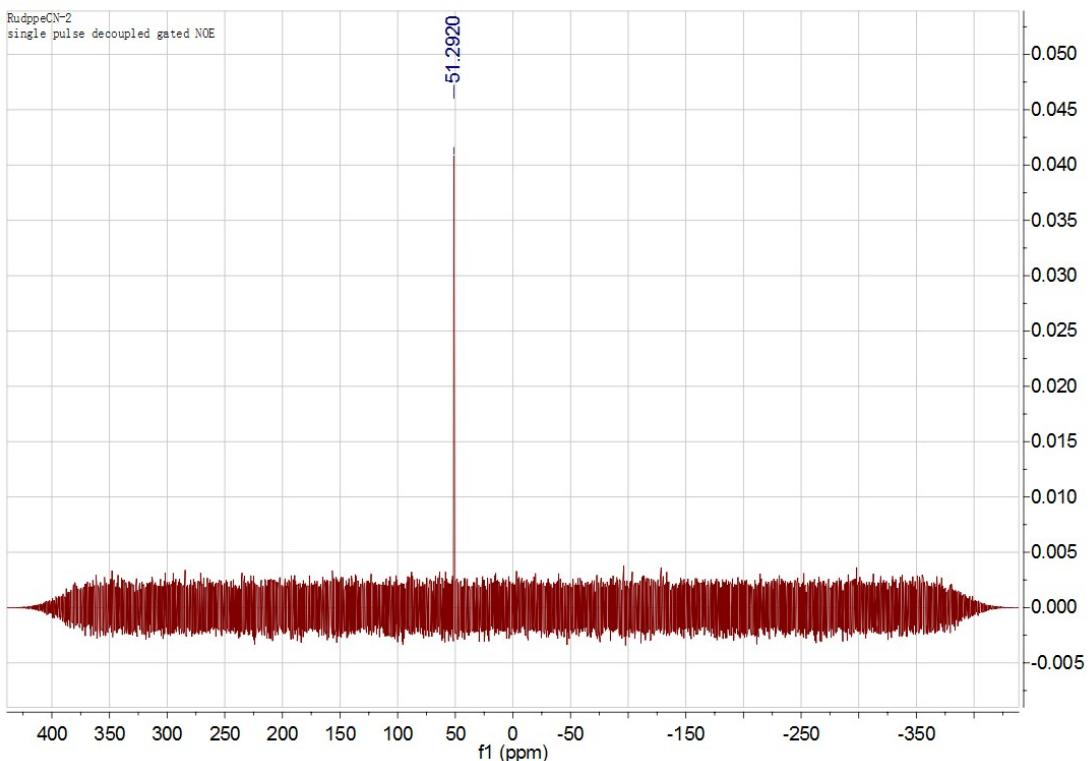


Figure S8 ^{31}P NMR of complex **1** in CDCl_3