Supporting Information

Syntheses, Structural and Serum Protein Protecting activity of Ruthenium(II)-DMSO complexes containing mercapto ligand

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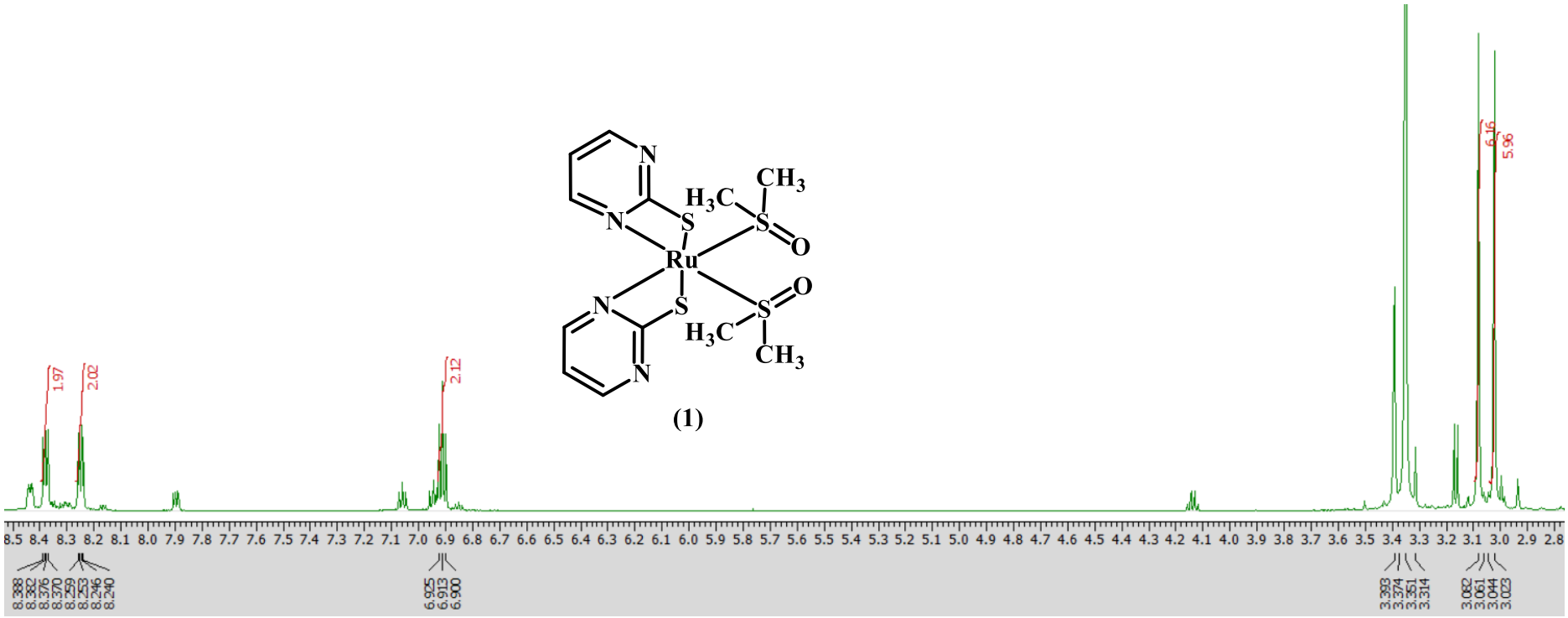
Content

NMR data for compounds



(ppm)

Figure S1. ^{1}H NMR spectrum of [Ru(mpt)$_2$(dmso)$_2$] (**1**) in DMSO-d_6 at 298K.

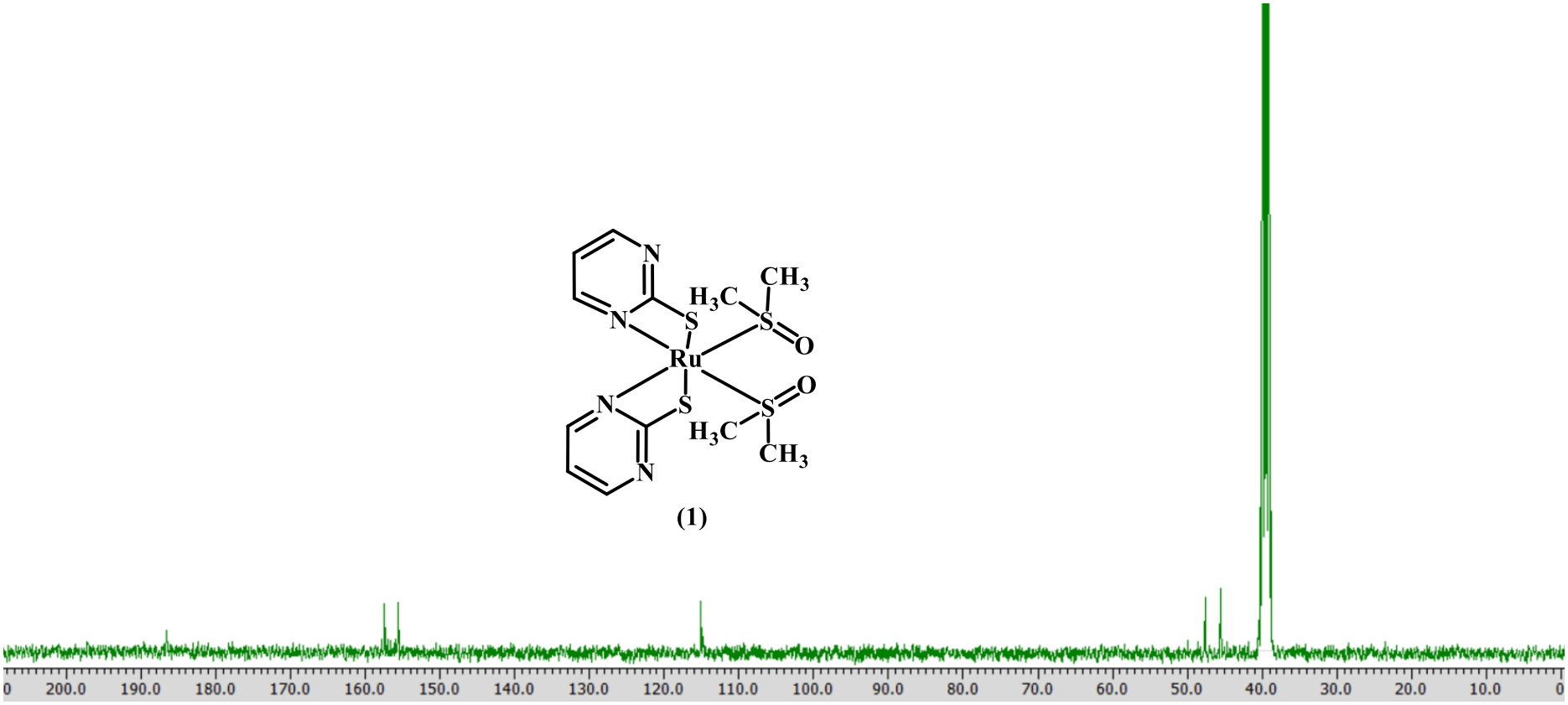


Figure S2. ^{13}C {^{1}H} NMR spectrum of [Ru(mpt)$_2$(dmso)$_2$] (**1**) in DMSO-d_6 at 298K.

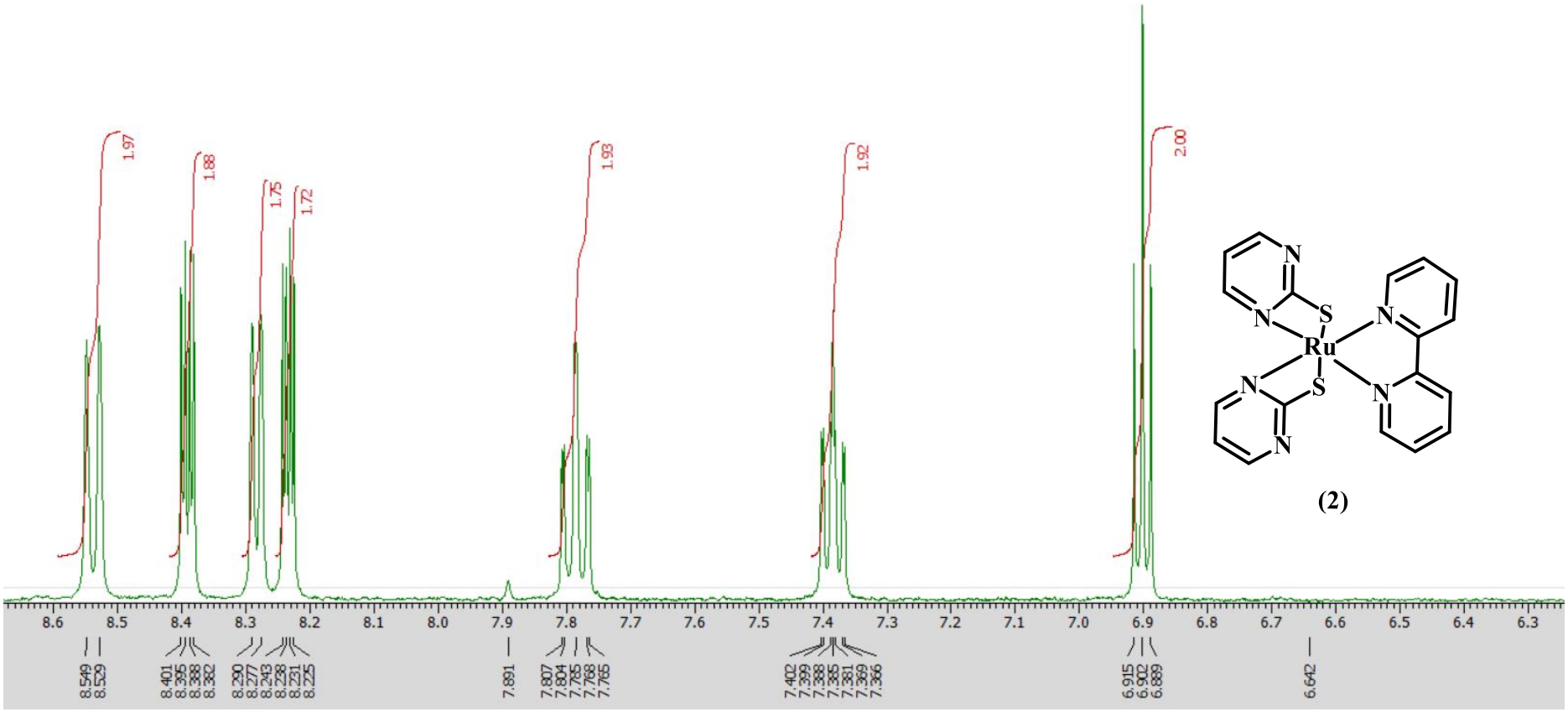
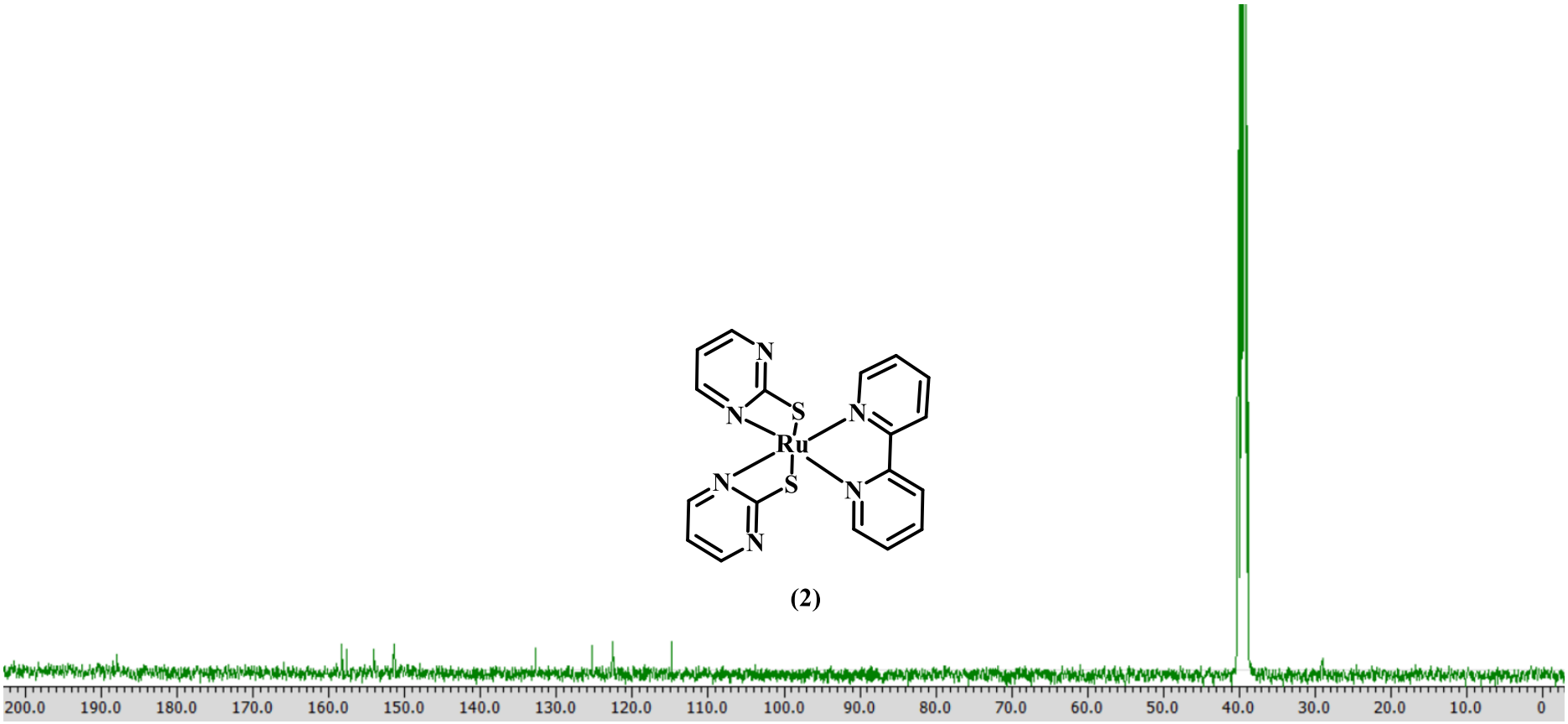


Figure S3. ^{1}H NMR spectrum of [Ru(mpt)$_2$(bpy)] (**2**) in DMSO-d_6 at 298K.



(2)

Figure S4. ^{13}C {^{1}H} NMR spectrum of [Ru(mpt)$_2$(bpy)] (**2**) in DMSO-d_6 at 298K.

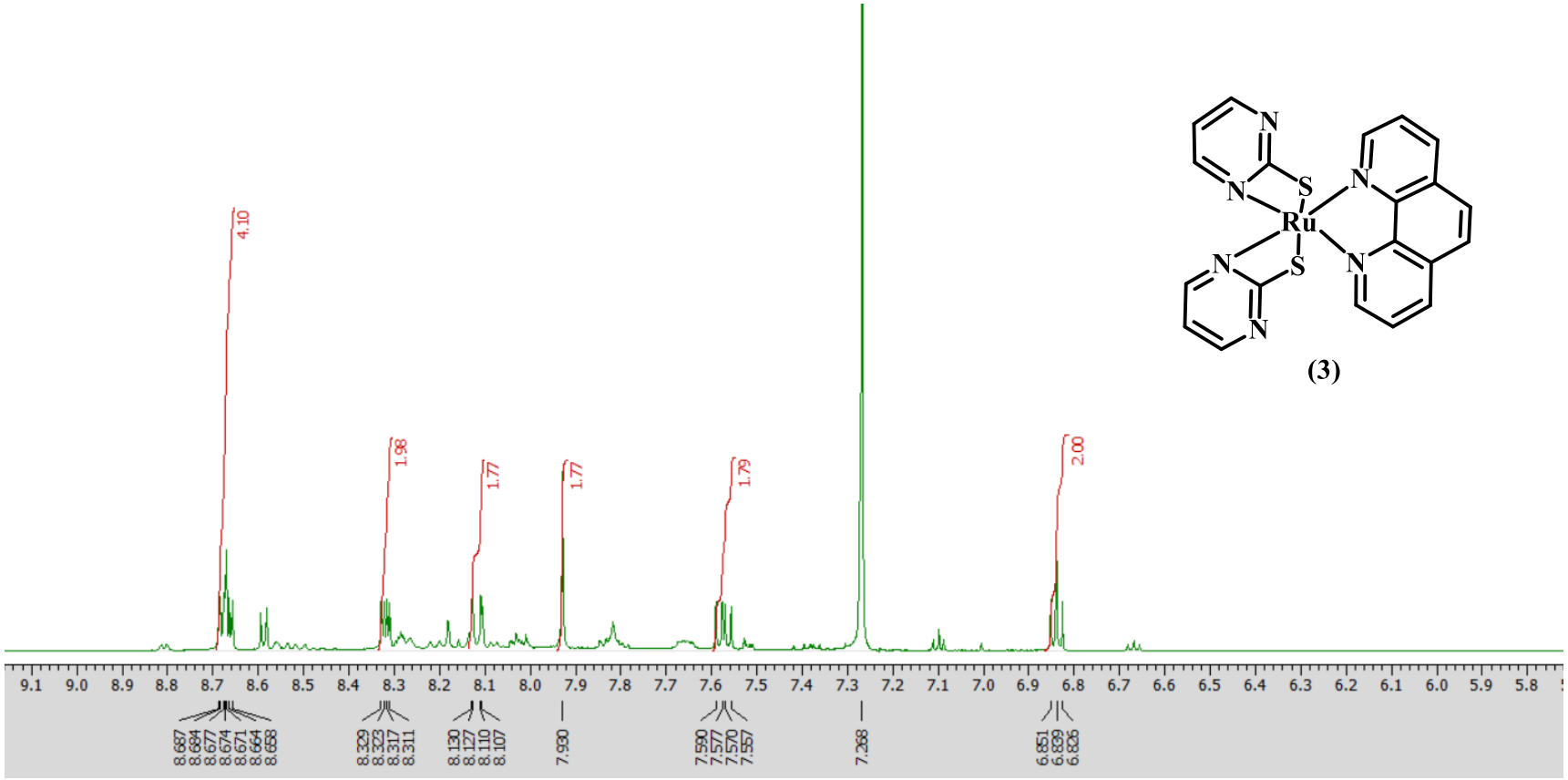


Figure S5. ^{1}H NMR spectrum of $[Ru(mpt)_2(Phen)]$ (**3**) in $CDCl_3$ at 298K.

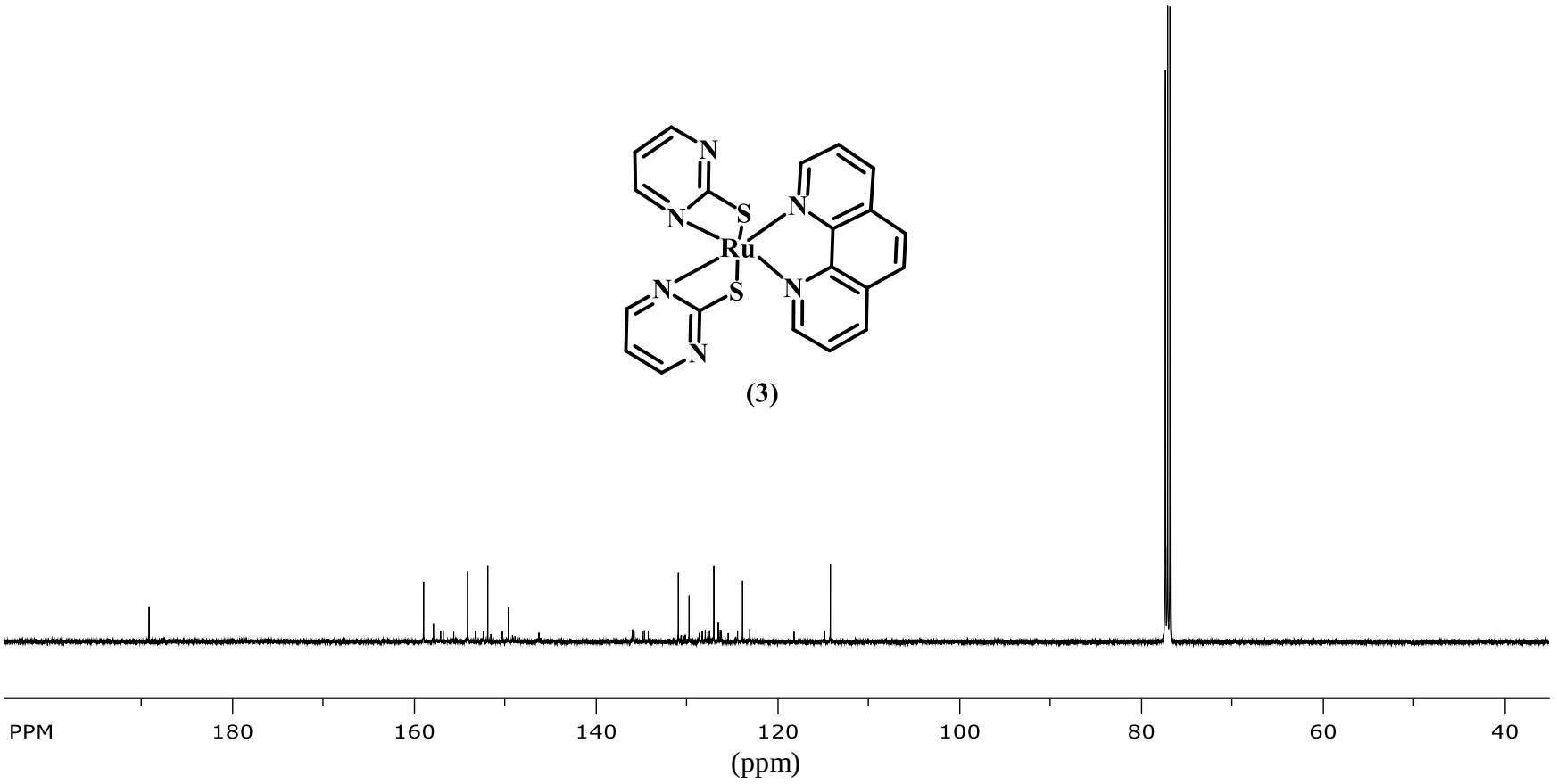


Figure S6. ^{13}C {^{1}H} NMR spectrum of [Ru(mpt)$_2$(Phen)] (**3**) in $CDCl_3$ at 298K.

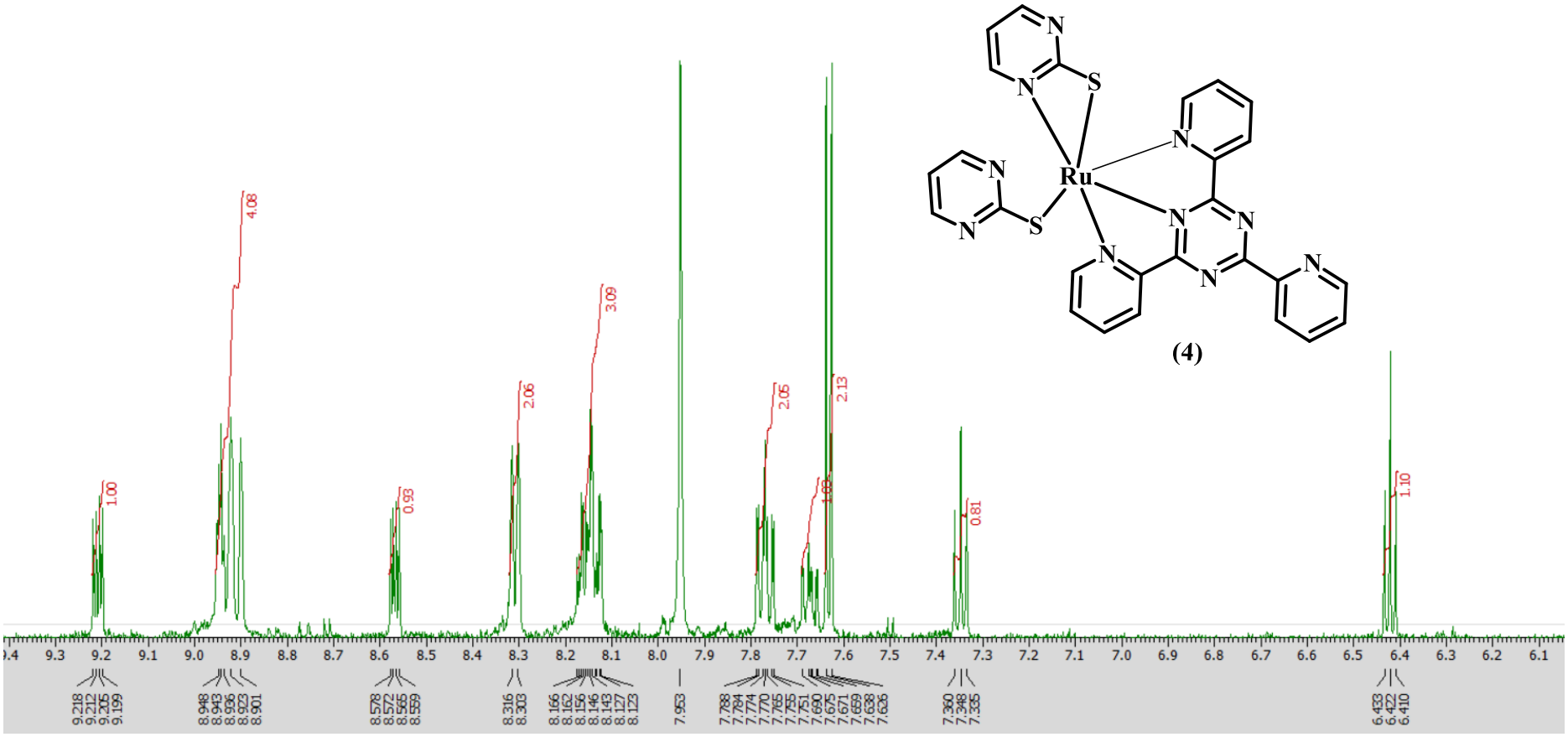


Figure S7. ^{1}H NMR spectrum of [Ru(mpt)$_2$(tptz)] (**4**) in $CDCl_3$ at 298K.

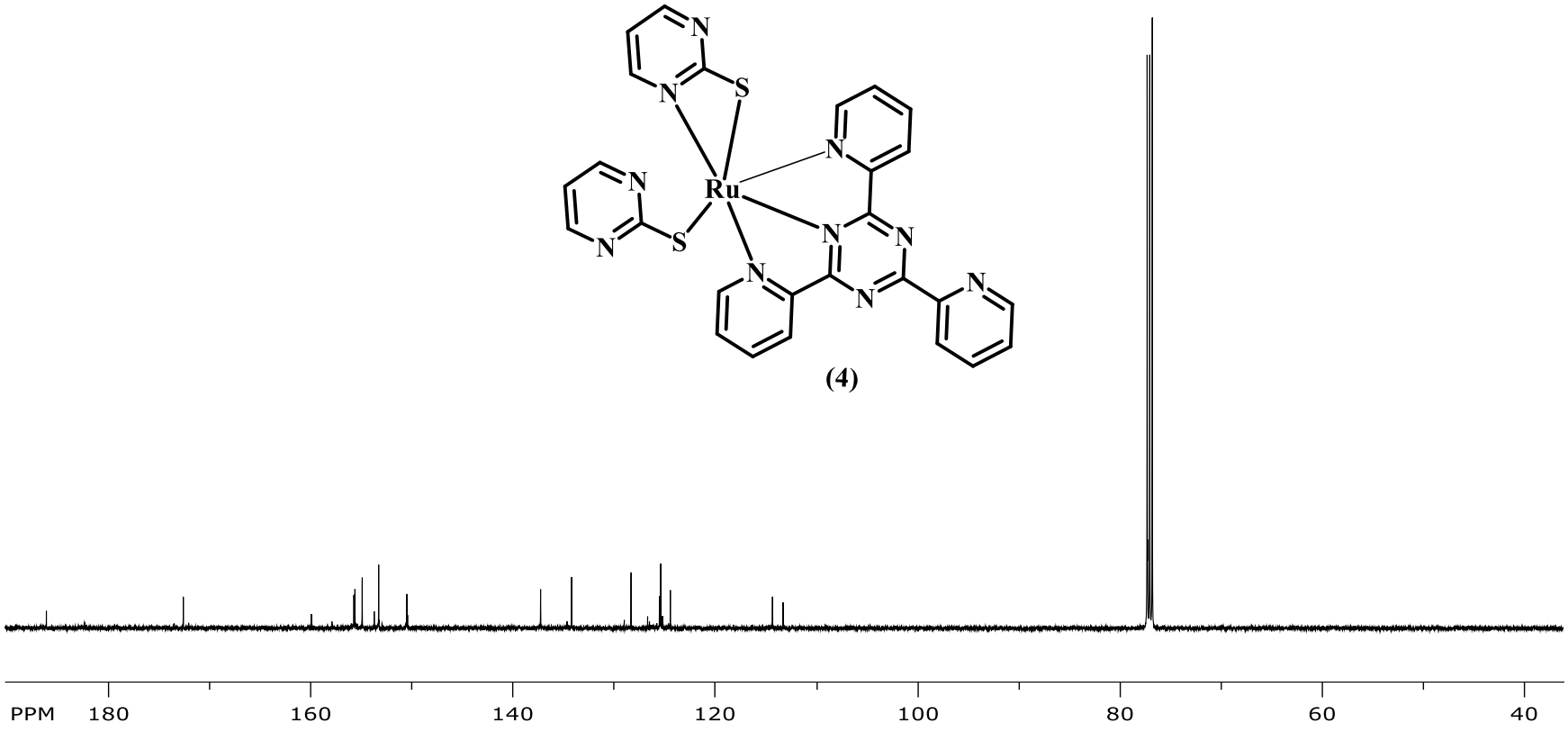


Figure S8. ^{13}C {^{1}H} NMR spectrum of [Ru(mpt)$_2$(tptz)] (**4**) in $CDCl_3$ at 298K.

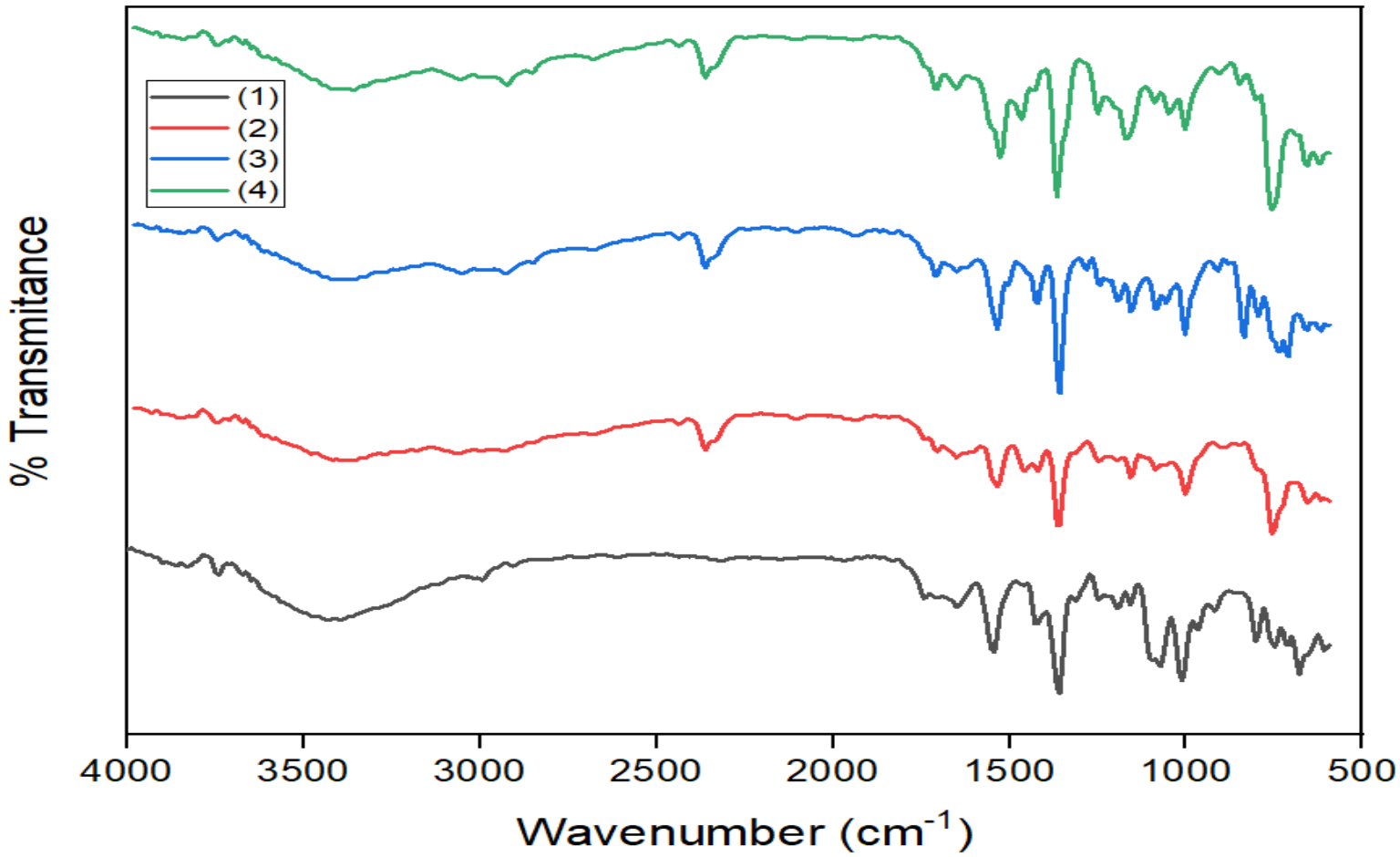


Figure S9. FTIR spectra of complexes **1-4**.

Table 1. Crystallographic data for complexes **1, 2** and **4**.

	1	**2**	**4**
empirical Formula	$C_{12}H_{18}N_4O_2S_4Ru$	$C_{18}H_{14}N_6S_2Ru$	$C_{26}H_{18}N_{10}S_2Ru$ [+solvent]
Fw	479.61	479.54	635.69
crystal system	Orthorhombic	Monoclinic	Monoclinic
space group	*Pbca*	$P2_1/c$	$P2_1/n$
a, Å	15.7042(2)	12.707(3)	9.05910(10)
b, Å	9.35780(10)	9.5980(19)	16.1092(2)
c, Å	25.3944(3)	14.964(3)	18.9209(2)
α, deg	90	90	90
β, deg	90	91.51(3)	100.5500(10)
γ, deg	90	90	90
V, $Å^3$	3731.88(8)	1824.4(7)	2714.54(5)
Z	8	4	4
d_{calc}, g cm^{-3}	1.707	1.746	1.555
μ, mm^{-1}	1.299	1.104	0.768
T, K	566(2)	566(2)	566(2)
R_1 all	0.0290	0.0234	0.0378
R_1 [I > 2σ(I)]	0.0233	0.0212	0.0283
wR_2	0.0571	0.0550	0.0724
wR_2 [I > 2σ(I)]	0.0545	0.0539	0.0680
GOF on F^2	1.043	1.042	1.062

Table 2. Hydrogen bonds for **1** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(4)-H(4)...O(1)	0.93	2.54	3.227(3)	130.9
C(4)-H(4)...O(1)#1	0.93	2.60	3.099(3)	114.3
C(11)-H(11A)...O(1)#1	0.96	2.41	3.355(3)	166.9
#C7-H(7)...S(2)#2	0.93	2.97	3.769(2)	144.4
#C7-H(7)...S(1)#3	0.93	3.01	3.586(3)	121.5
C(2)-H(2)...O(2)#4	0.93	2.53	3.264(3)	136.1
C(9)-H(9A)...O(2)	0.96	2.41	3.148(4)	133.6
#C9-H(9C)...S(2)	0.96	3.00	3.540(3)	117.3
#C10-H(10B)...S(1)#5	0.96	2.96	3.868(3)	158.8
#C12^a-H(12B^a)...S(1)	0.96	2.95	3.545(18)	121.1
C(12'^b)-H(12D^b)...N(4)#6	0.96	2.59	3.33(2)	133.8

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 x-1/2,y,-z+3/2 #3 -x+1/2,y-1/2,z

#4 x-1/2,-y+3/2,-z+1 #5 x,y-1,z #6 -x+1,y+1/2,-z+3/2

Table 3. Hydrogen bonds for **2** [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
C(8)-H(8)...S(1)#1	0.93	3.00	3.705(2)	133.6
C(8)-H(8)...N(4)#1	0.93	2.58	3.388(3)	146.1
C(9)-H(9)...N(3)	0.93	2.63	3.161(3)	117.2
C(10)-H(10)...N(4)#2	0.93	2.65	3.486(3)	149.2
C(17)-H(17)...S(2)#3	0.93	2.85	3.616(2)	139.8
C(18)-H(18)...N(5)	0.93	2.69	3.187(3)	114.6

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y+1/2,-z+3/2 #2 -x+1,y-1/2,-z+3/2 #3 -x+2,y+1/2,-z+3/2