Atom-economical Synthesis of the Versatile Ruthenium Precursor [TpRuCl(COD)] (Tp = hydrotris(pyrazol-1-yl)borate) Discloses a Diamine Ligand Dealkylation Process

Manuel Jiménez-Tenorio, M. Carmen Puerta* and Pedro Valerga*

Departamento de Ciencia de los Materiales e Ingeniería Metalúrgica y Química Inorgánica-INBIO, Facultad de Ciencias, Universidad de Cádiz, 11510 Puerto Real, Cádiz, Spain

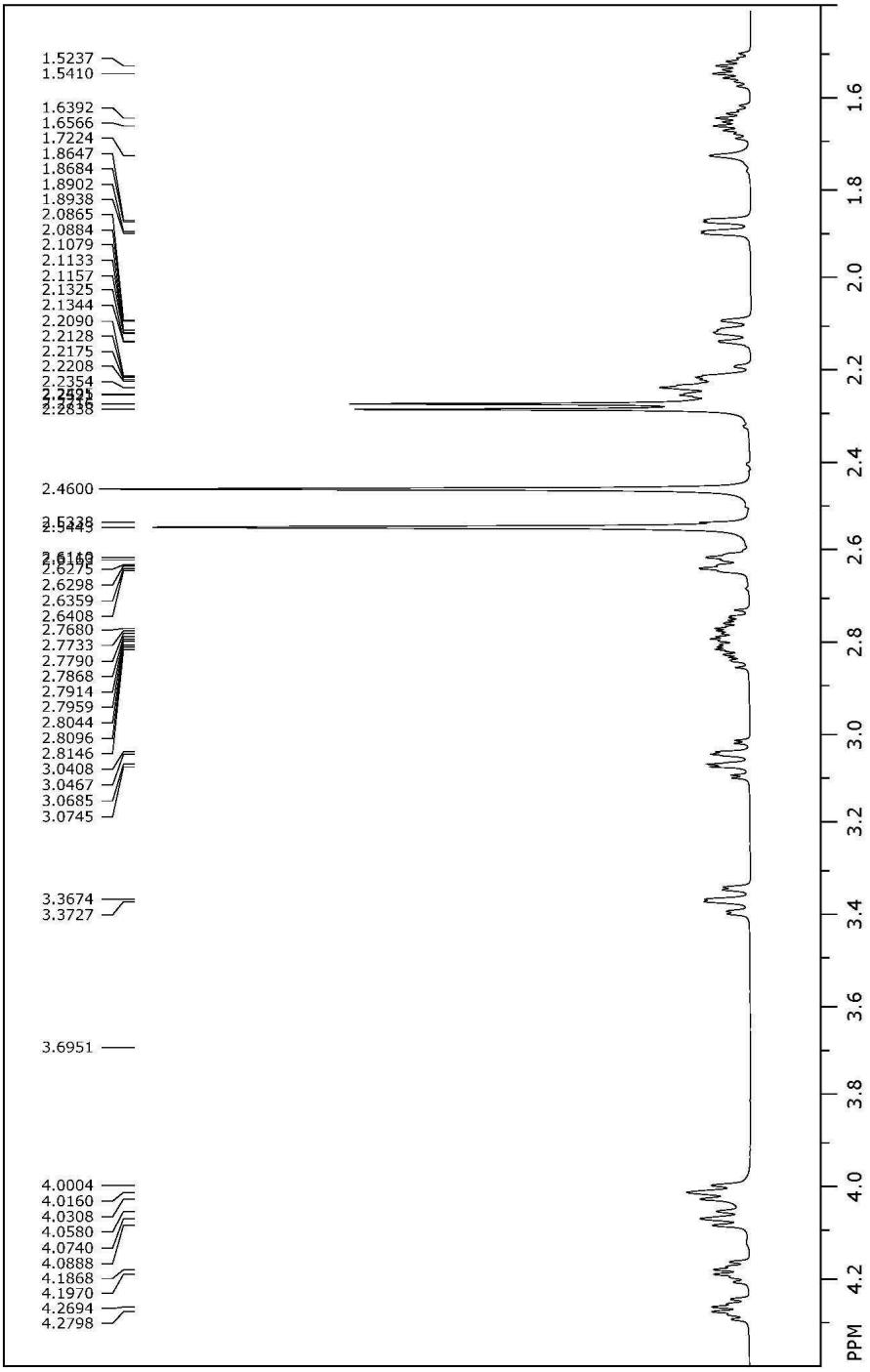
SUPPORTING INFORMATION:

1. Table S1: Crystal data and experimental details for the crystal structure determination of 2.

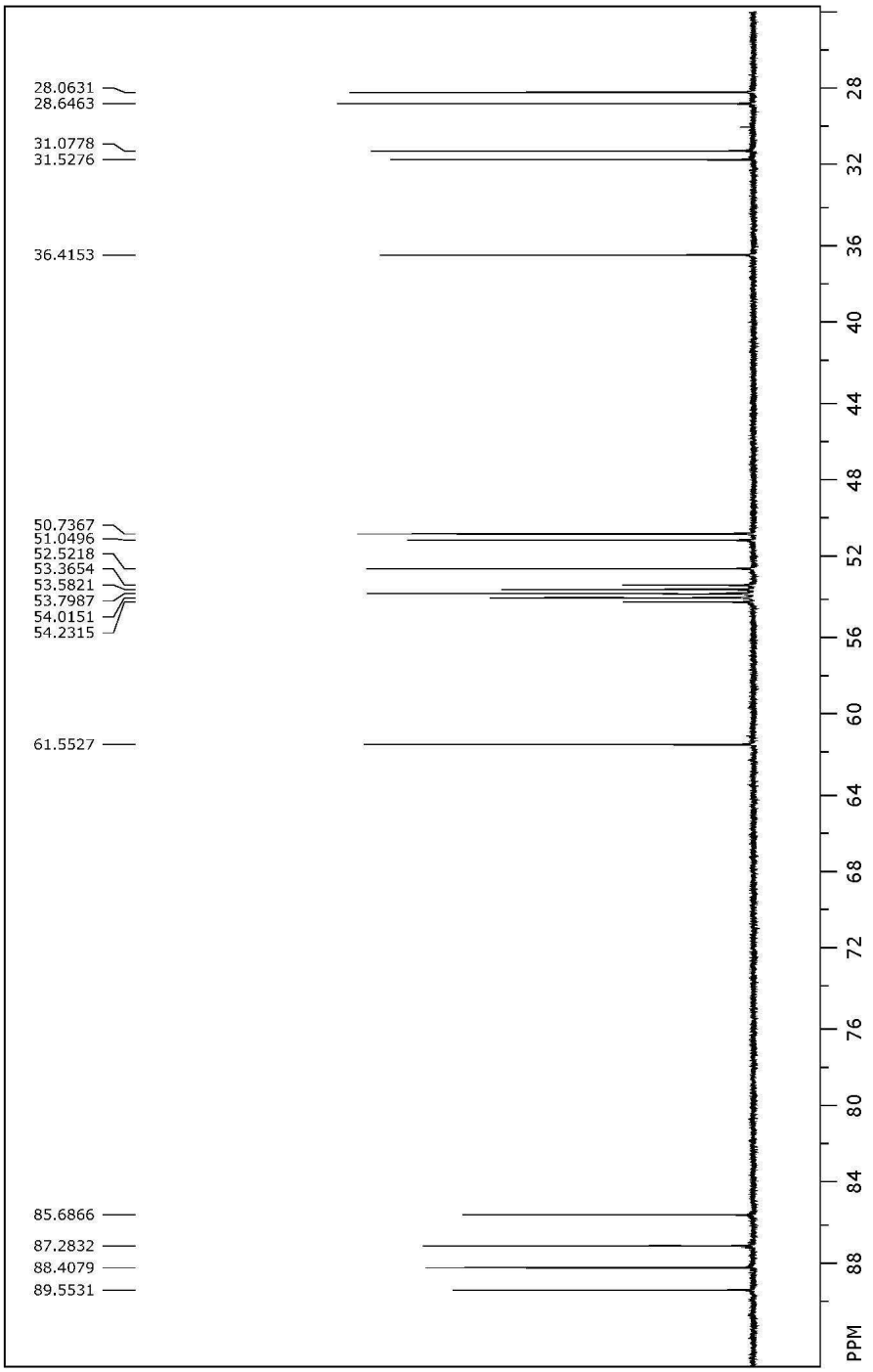
Compound	**2**
Formula	$C_{13}H_{26}Cl_2N_2Ru$
FW	382.33
T (K)	100(2)
Crystal size (mm)	0.38 x 0.19 x 0.08
Crystal system	Monoclinic
Space group	C 2/*c* (no. 15)
Cell parameters	*a* = 25.543(5) Å
	b = 8.7306(17) Å
	c = 14.199(3) Å
	α = 90.00
	β = 104.11(3)
	γ = 90.00
Volume (Å^3)	3070.9(11)
Z'	8
ρ_{calc} (g cm^{-3})	1.654
μ(Mo Kα) (mm^{-1})	1.355
F(000)	1568
Max. and min. transmission factors	1.000-0.850
Theta range for data collection	1.64 < θ < 27.53
Reflections collected	12396
Unique reflections	3535

	(R_{int} = 0.0296)
No. of observed reflections ($I > 2\sigma_I$)	3386
No. of parameters	166
Final R1, wR2 values ($I > 2\sigma_I$)	0.0254, 0.0580
Final R1, wR2 values (all data)	0.0273, 0.0593
Residual electron density peaks (e $Å^{-3}$)	+0.103, -0.749

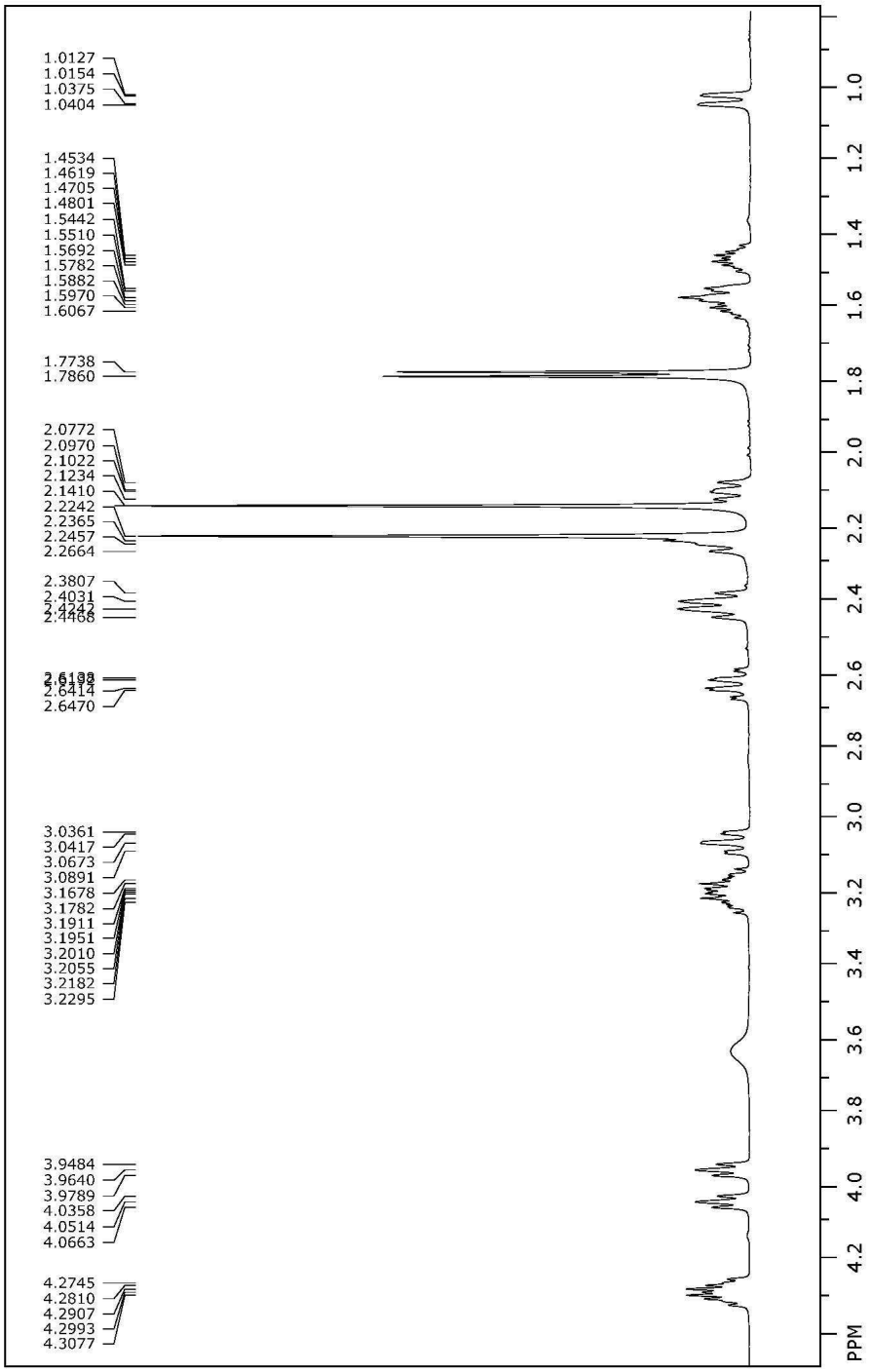
2. Figure S1: ^{1}H NMR spectrum of 2 in CD_2Cl_2



3. Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of 2 in CD_2Cl_2



4. Figure S3: ^{1}H NMR spectrum of 2 in C_6D_6



5. Figure S4: 2D ^{1}H-gCOSY NMR spectrum of 2 in C_6D_6