Electronic Supplementary Information

Novel class of Bi(III) hydroxamato complexes: synthesis, urease inhibitory activity and activity against *H. pylori*

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Contents:

Table 1 Crystallographic data for 1 and 2.

	1	**2**
Empirical formula	C29 H28 Bi2 N6 O15	C90 H108 Bi6 N18 O66
Formula weight	1118.53	3751.82
Temperature	100(2) K	100(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Triclinic	Triclinic
Space group	$P\bar{1}$	$P\bar{1}$
Unit cell dimensions	a = 4.8467(4) Å	a = 15.0432(6) Å
α= 112.5660(10)°.		
	b = 13.1798(12) Å	b = 15.2366(5) Å
β= 116.5850(10)°.		
	c = 15.0042(14) Å	c = 16.5434(6) Å
γ = 94.4850(10)°.		
Volume	913.72(14) $Å^3$	2984.48(19) $Å^3$
Z	1	1
Density (calculated)	2.033 Mg/m^3	2.087 Mg/m^3
Absorption coefficient	9.692 mm^{-1}	8.926 mm^{-1}
F(000)	530	1800
Crystal size	0.210 x 0.050 x 0.030 mm^3	0.150 x 0.080 x 0.050 mm^3
Theta range for data collection	1.412 to 27.534°.	1.518 to 30.135°.
Index ranges	-6≤h≤6, -17≤k≤17, -19≤l≤19	-21≤h≤21, -21≤k≤21, -23≤l≤23
Reflections collected	32284	111802
Independent reflections	4213 [R(int) = 0.0626]	17529 [R(int) = 0.0443]
Completeness to theta = 25.242°	100.0 %	100.0 %
Absorption correction	Semi-empirical from equivalents	Numerical
Max. and min. transmission	0.7456 and 0.4625	0.7837 and 0.4747
Refinement method	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	4213 / 94 / 251	17529 / 14 / 827
Goodness-of-fit on F^2	1.084	1.004
Final R indices [I>2σ(I)]	R1 = 0.0371, wR2 = 0.0904	R1 = 0.0254, wR2 = 0.0489

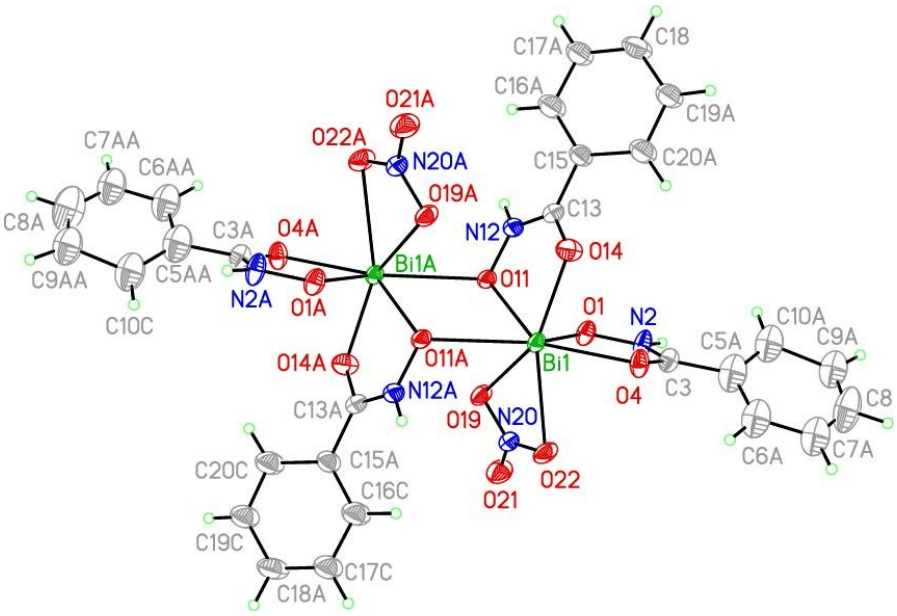
R indices (all data)	R1 = 0.0437, wR2 = 0.0935	R1 = 0.0411, wR2 = 0.0533
Largest diff. peak and hole	2.302 and -1.477 e.Å^{-3}	1.894 and -1.451 e.Å^{-3}

Table 2. Coordination Geometry around Bi centres for 1 and 2.

Bond	Distance (Å)	Bond	Distance (Å)	Bond	Distance (Å)
1					
Bi1-O1	2.201(5)				
Bi1-O11	2.234(4)				
Bi1-O14	2.276(5)				
Bi1-O4	2.409(5)				
Bi1-O19	2.519(5)				
Bi1-O11$^{\$1}$	2.674(5)				
Bi1-O22	2.755(5)				
Bi1-O1$^{\$2}$	3.034(5)				
2					
Bi1-O10	2.256(2)	Bi2-O5	2.604(3)	Bi3-O2	2.515(3)
Bi1-O11	2.327(2)	Bi2-O6	2.509(3)	Bi3-O3	2.893(4)
Bi1-O14	2.773(3)	Bi2-O32	2.230(2)	Bi3-O10$^{\$3}$	2.721(2)
Bi1-O21	2.337(2)	Bi2-O33	2.277(2)	Bi3-O21$^{\$3}$	3.201(3)
Bi1-O21$^{\$3}$	2.577(2)	Bi2-O43	2.459(2)	Bi3-O43	2.427(2)
Bi1-O22	2.269(2)	Bi2-O44	2.312(3)	Bi3-O54	2.329(2)
Bi1-O32	2.521(2)	Bi2-O54	2.639(2)	Bi3-O55	2.378(3)
Bi1-O43	2.829(2)	Bi2-O65	2.822(2)	Bi3-O65	2.226(2)
Bi1-O54	3.158(2)			Bi3-O66	2.380(2)

Symmetry transformations used to generate equivalent atoms: $1 = -x+1,-y+1,-z; $2 = 1+x, y, z; $3 = -x+1,-y+1,-z+1

A



B

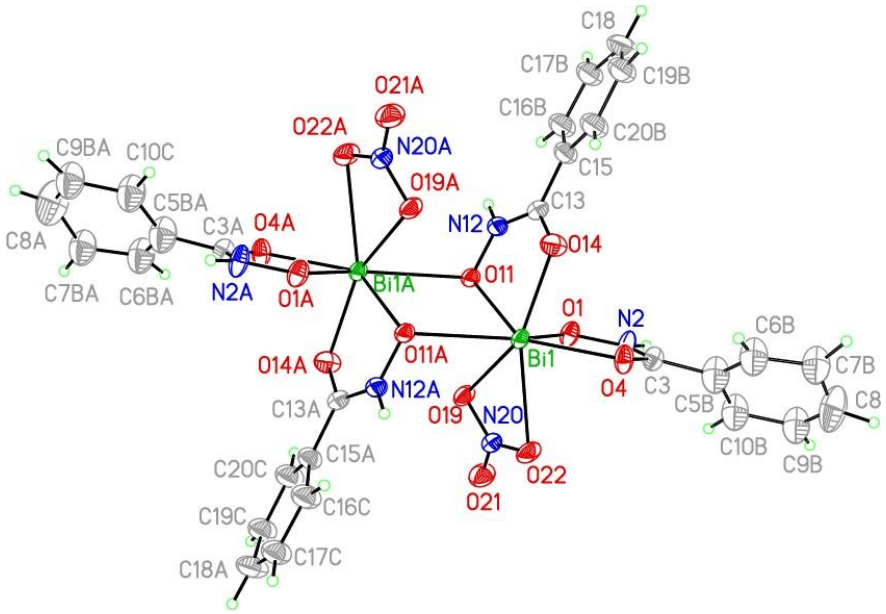


Fig S1. Structure of 1 showing both disordered (A, 50; B, 50%) moieties with full atom labelling.

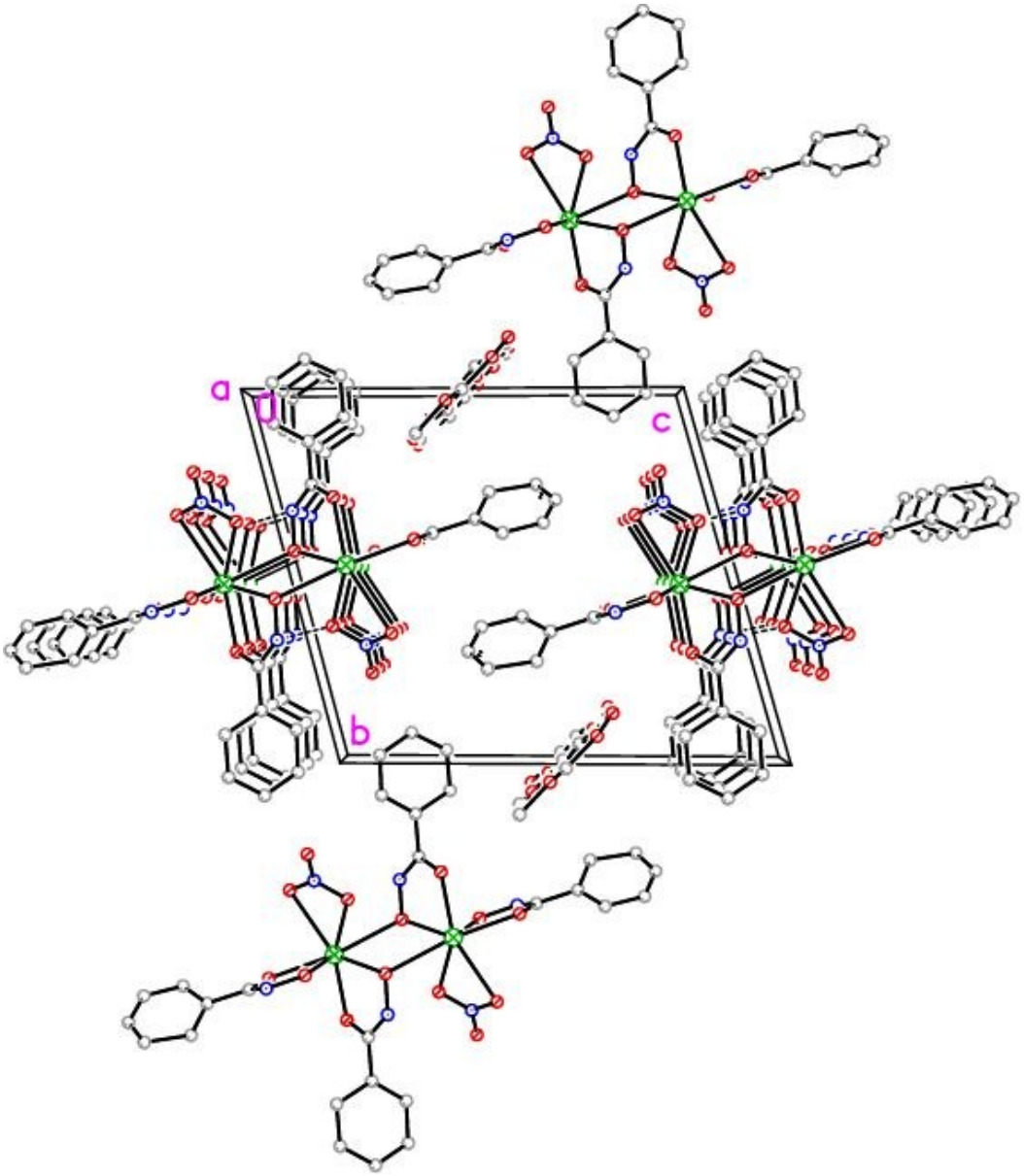


Fig. S2 Packing diagram of 1 (major moiety only) viewed down the a-axis. Disordered MeOH solvent included. Hydrogen atoms omitted for clarity.

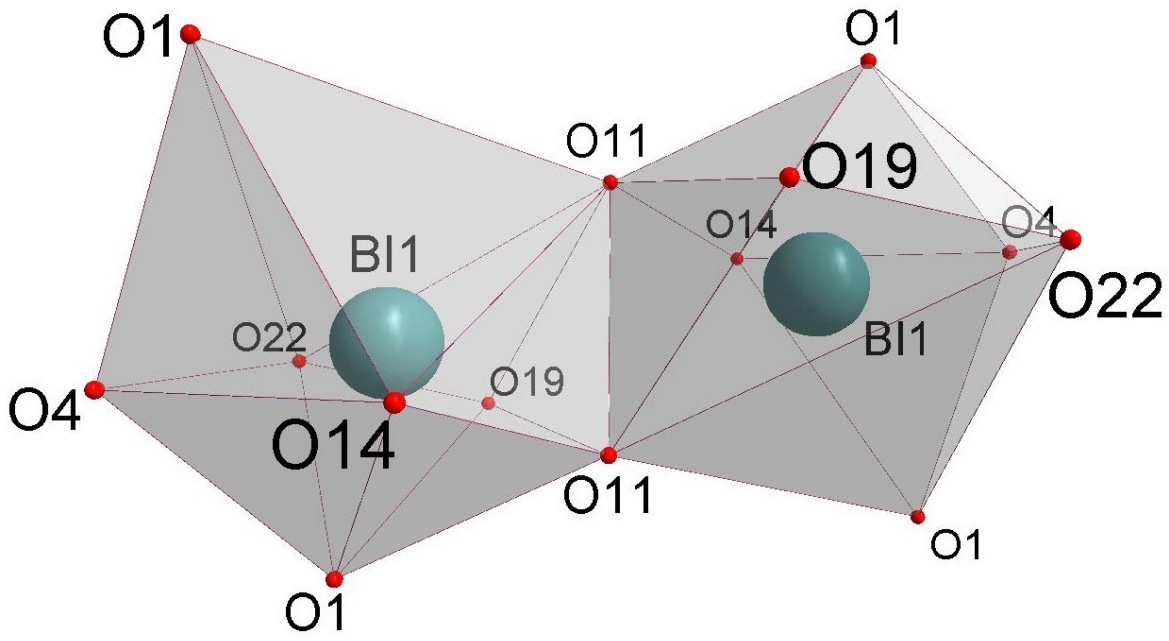


Fig. S3 Coordination geometry in 1 with atom labelling.

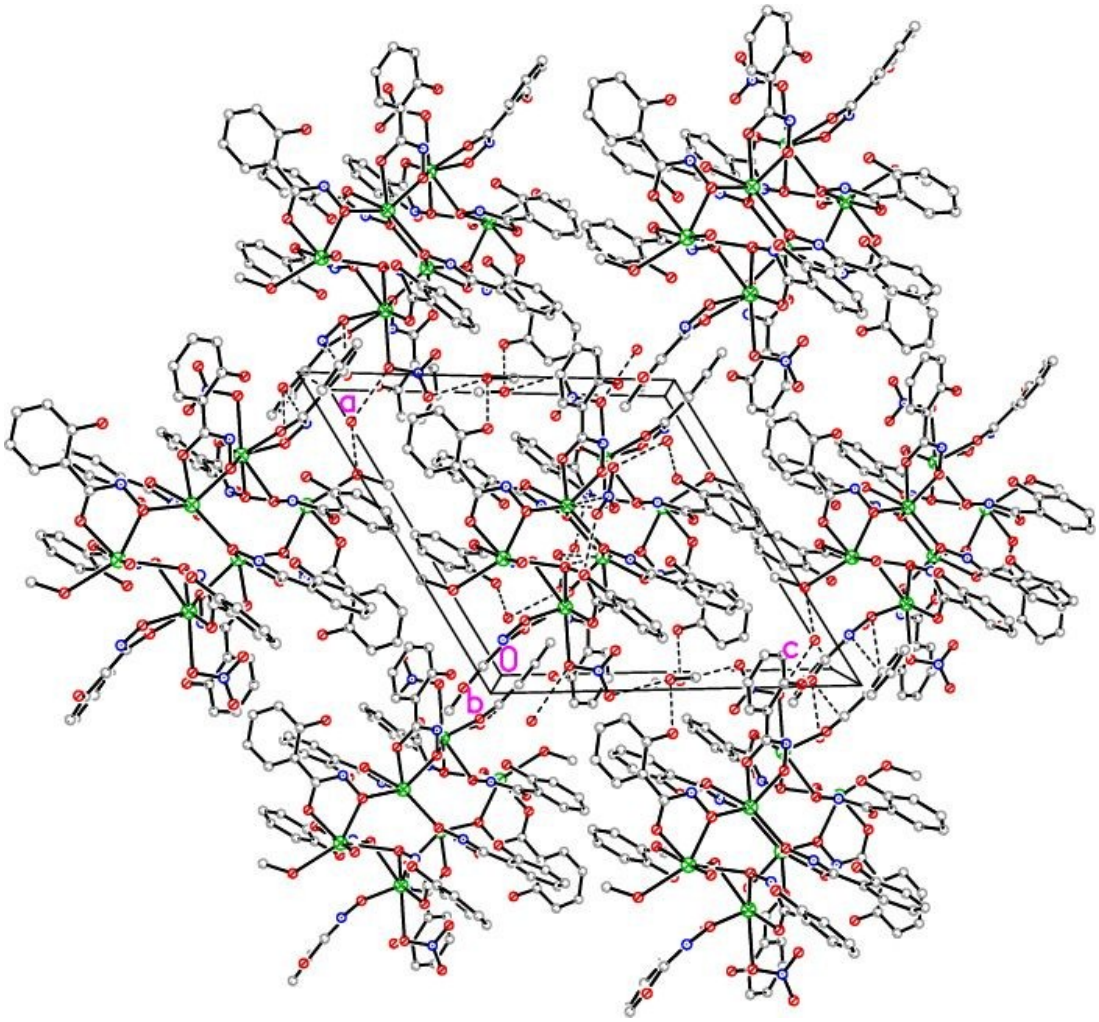


Fig. S4 Packing diagram of 2 viewed down the a-axis. Hydrogen atoms omitted for clarity. Dashed lines indicate strong hydrogen bonding.

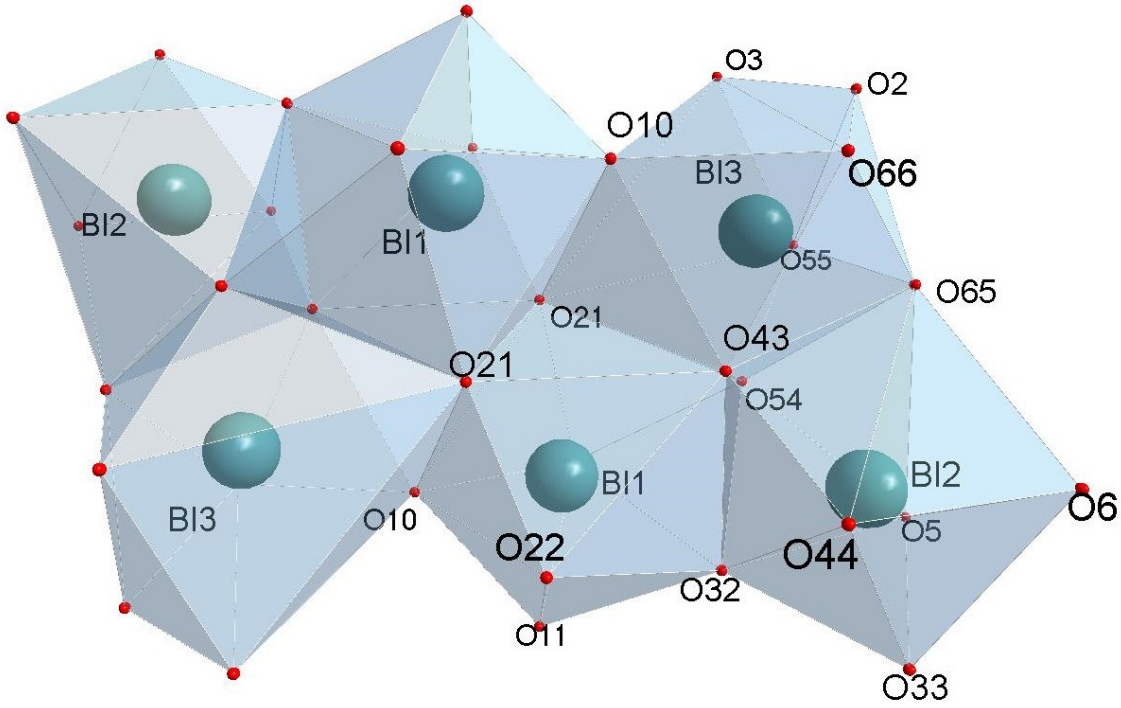


Fig. S5. Coordination geometry in 2 with atom labelling.

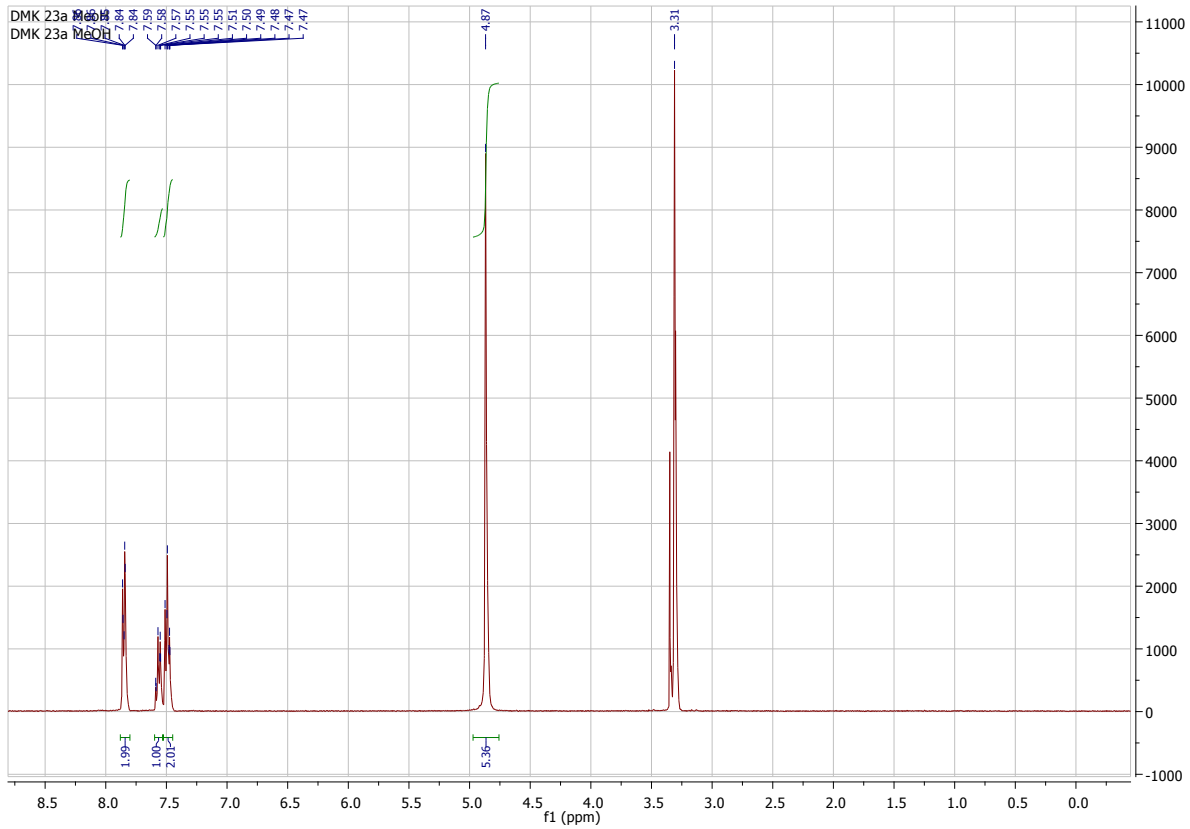


Fig. S6 ^{1}H NMR spectrum of complex 1.

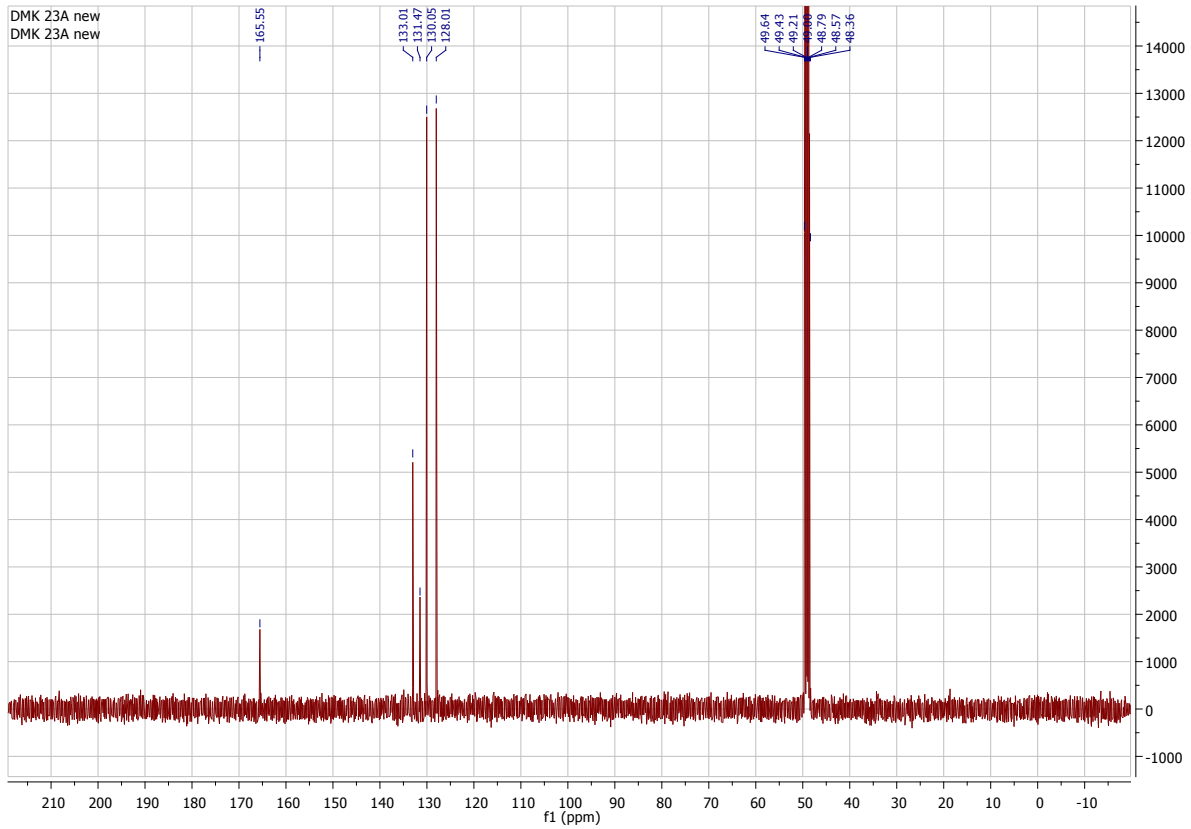


Fig. S7 ^{13}C NMR spectrum of complex 1.

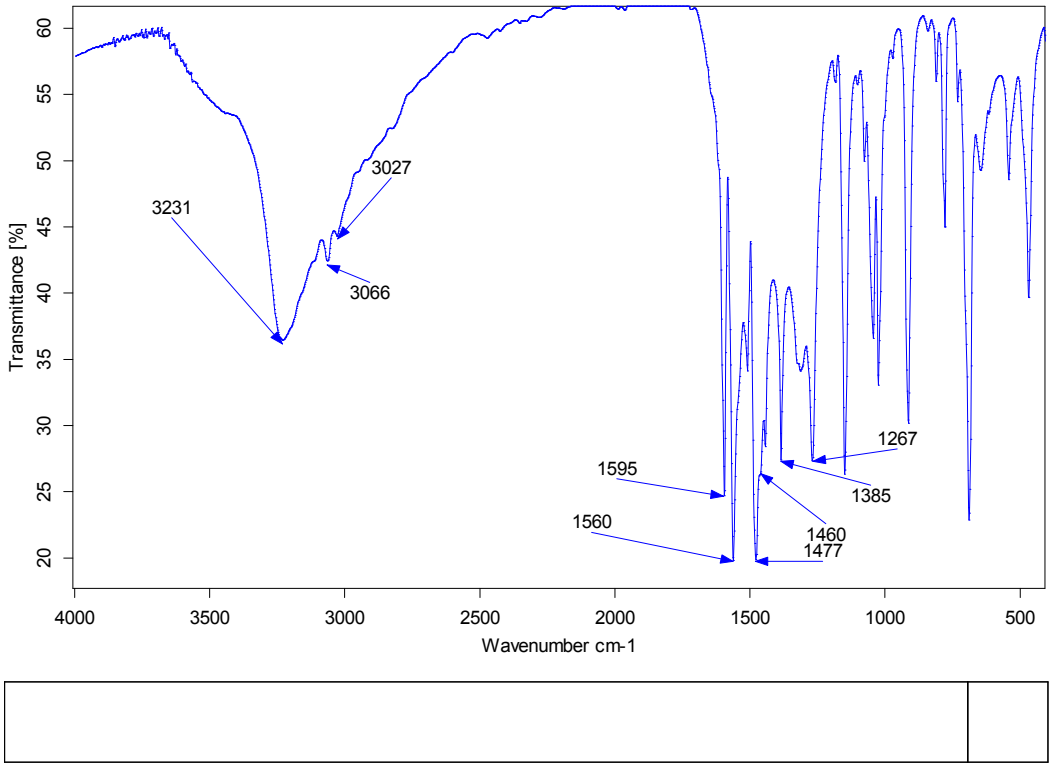


Fig. S8 FTIR spectrum of complex 1.

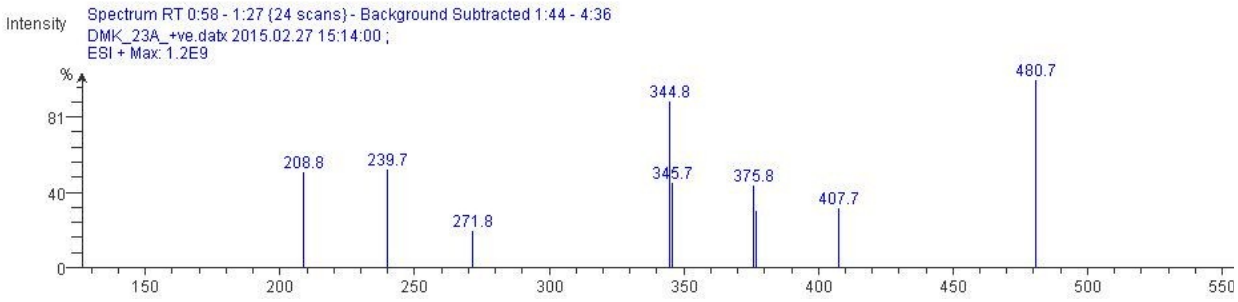


Fig. S9 ESI Mass Spectrum of Complex 1.