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Supporting information for article:

First heterobimetallic Ag^{I}–Co^{III} coordination compound with both bridging and terminal –NO2 coordination modes: synthesis, characterization, structural and computational studies of (PPh3)2Ag^{I}–(μ-κ^{2}*O*,*O*′;κ*N*-NO2–Co^{III}(DMGH)2(κ*N*-NO2)

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Supporting Information

First Heterobimetallic Ag^{I}-Co^{III} Coordination Compound with both Bridging and Terminal $–NO_2$ Coordination Modes: Synthesis, Characterization, Structural and Computational Studies of $(PPh_3)_2Ag^{I}$-(κ^2-O,O′-κ^1-N)NO_2-$Co^{III}(DMGH)_2(\kappa^1$-$NO_2)$

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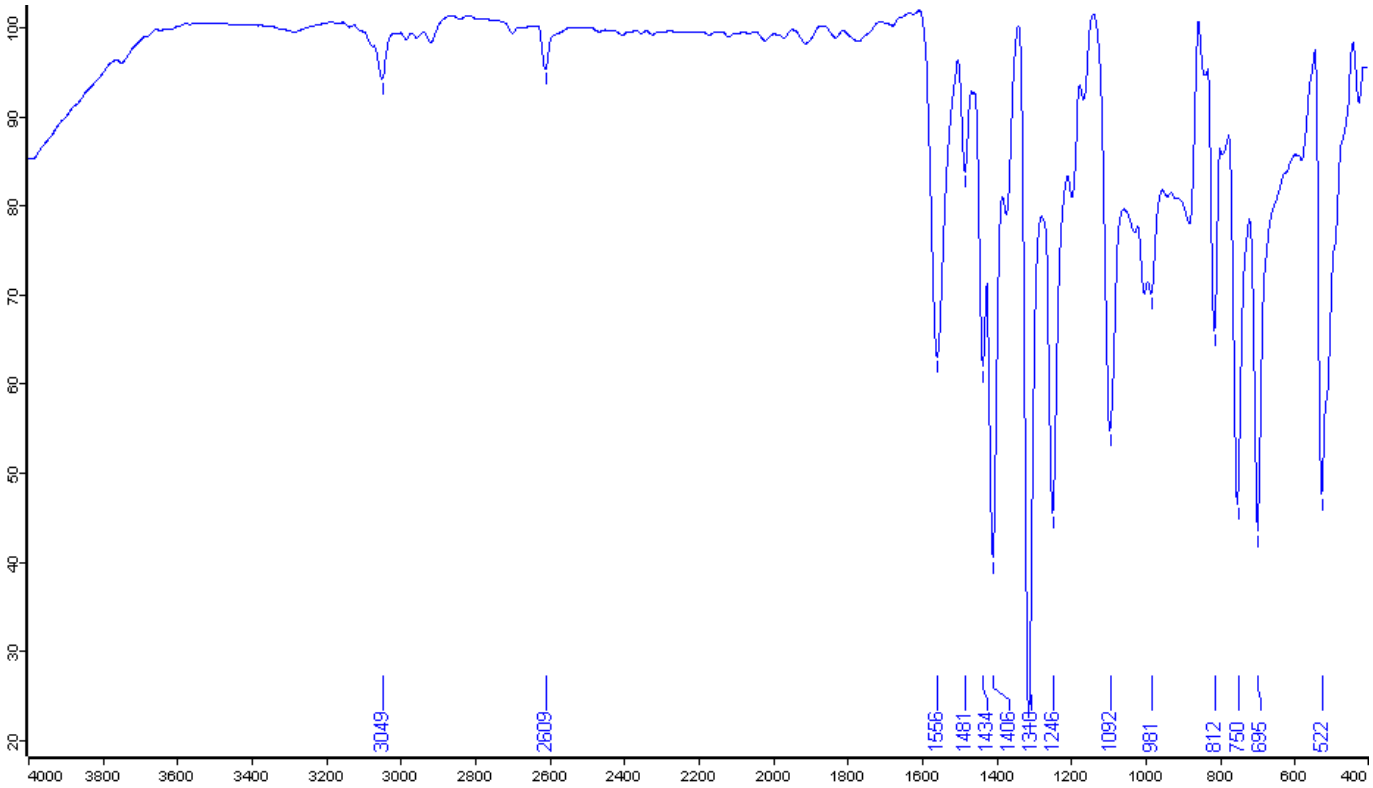

Fig. S1. The FT-IR spectrum of **1**.

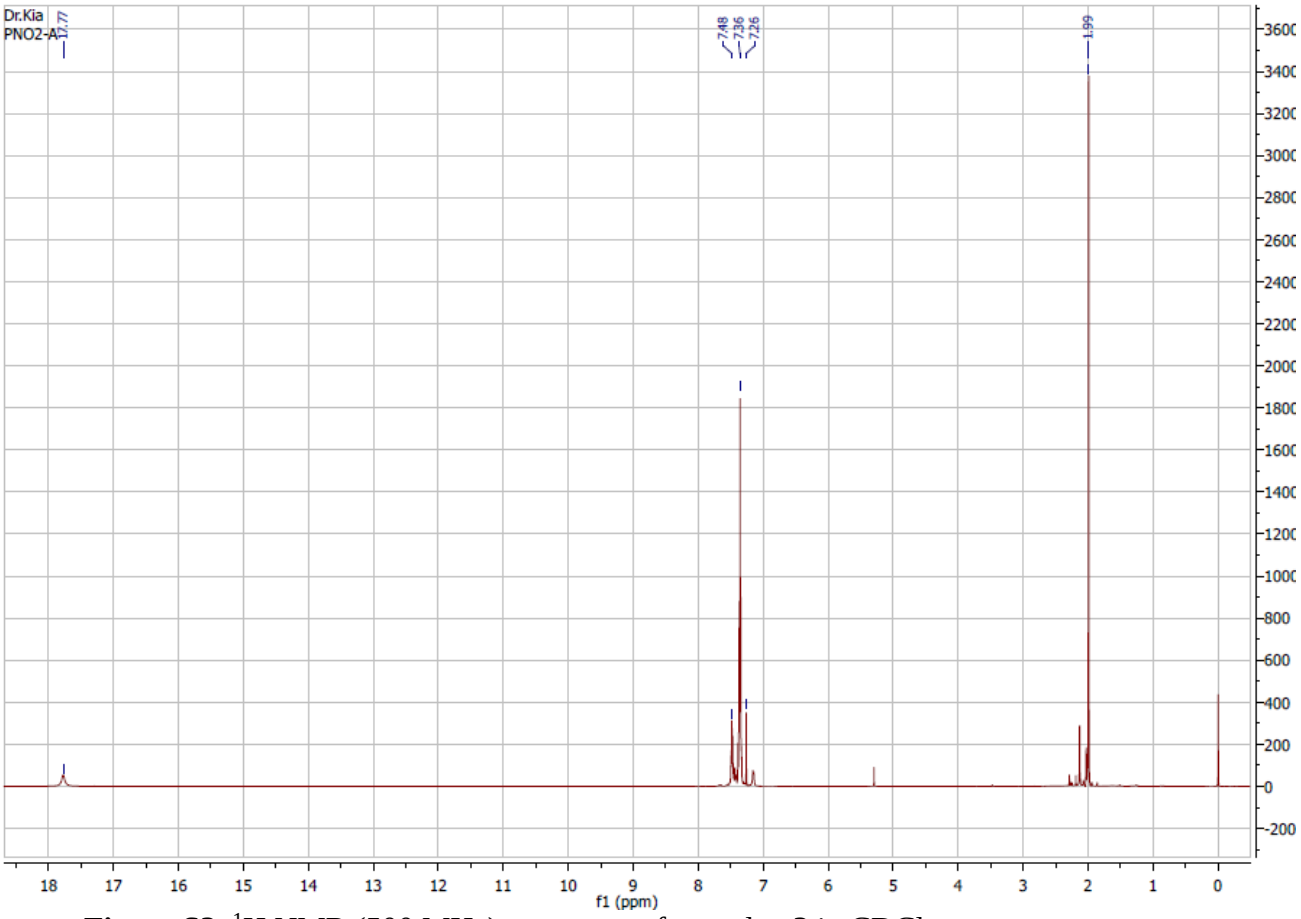

Figure S2. ^{1}H NMR (500 MHz), spectrum of complex **2** in $CDCl_3$ at room temperature.

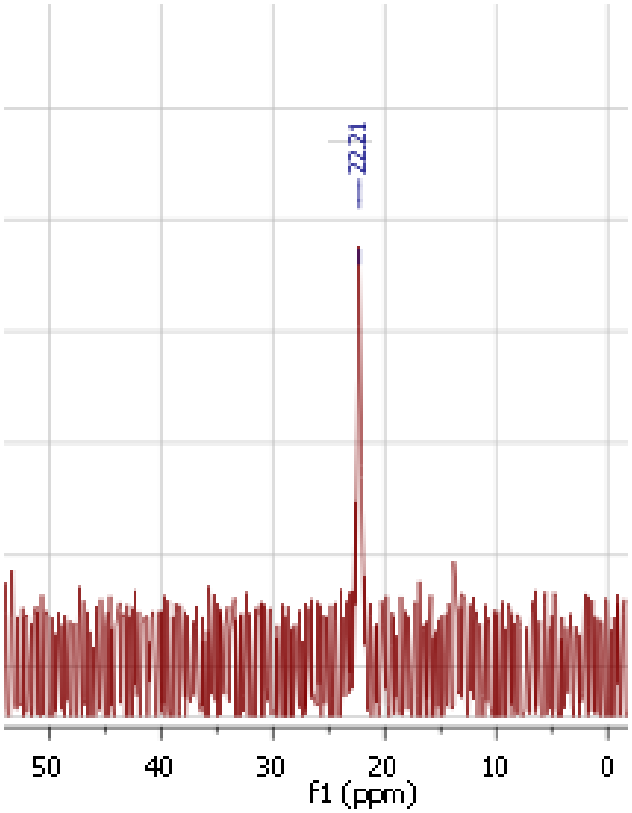

Fig. S3. ^{31}P {^{1}H} NMR spectrum of **1** in $CDCl_3$ at room temperature.

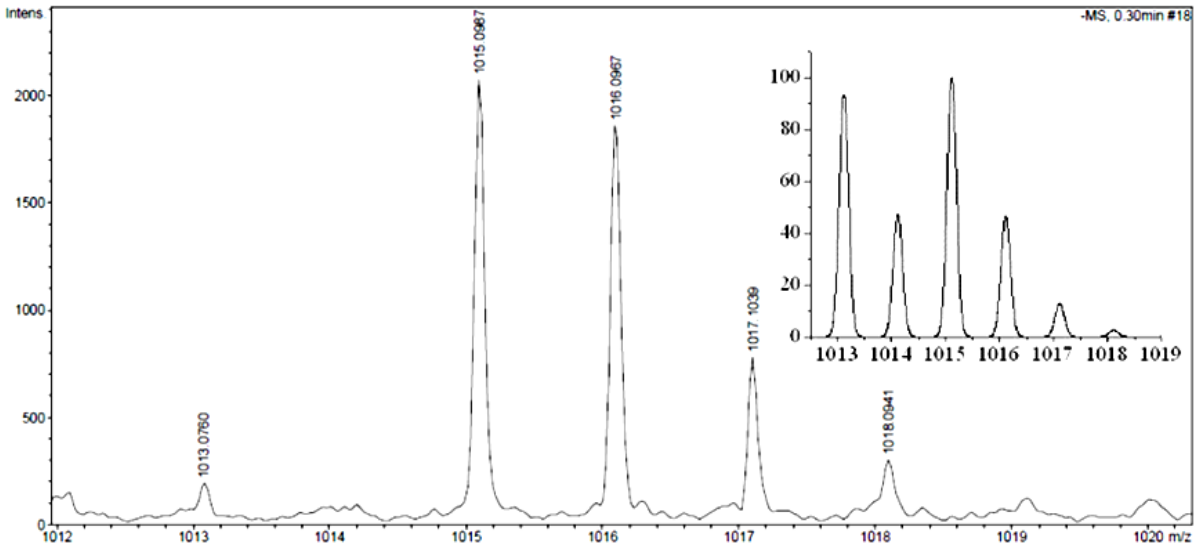

Fig. S4. Expanded ESI-MS spectrum of **1** in base peak position. Inset shows the simulated isotope pattern.

Table S1. G03/B3LYP calculated one-electron energy and percentage composition of selected frontier MOs of **1** expressed in terms of component fragments

MO	Name	E (eV)	Ag	PPh_3	NO_2[b]	Co	DMGH[c]	NO_2[t]
246	LUMO + 5	-1	4.1	90.8	4.6	0.2	0.4	0
245	LUMO + 4	-1.1	7	54.6	4.8	5.1	28.2	0.3
244	LUMO + 3	-1.1	6.6	79.2	1.7	6.7	5.2	0.7
243	LUMO + 2	-1.2	6.8	50.9	5.1	15.8	17.8	3.6
242	LUMO + 1	-1.2	4.5	95	0.4	0.1	0	0
241	**LUMO**	**-1.3**	**5.7**	**11.8**	**76**	**2.9**	**3.2**	**0.3**
240	**HOMO**	**-5**	**0.1**	**2.6**	**0.5**	**0.3**	**94.8**	**1.7**
239	HOMO – 1	-5.1	0.2	2	0.1	6.1	91.2	0.3
238	HOMO – 2	-5.7	3.9	3.8	15.4	13.1	3.6	60
237	HOMO – 3	-5.8	0.1	2	0.5	3.4	88.4	5.4
236	HOMO – 4	-6.2	0.4	0.4	3.1	2.5	25.2	68.5
235	HOMO – 5	-6.4	15.5	83.8	0.4	0.1	0	0

[b] Bridged NO2; [c] Dimethylglyoximate; [t] Terminal