Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

Vinylimidazole coordination modes to Pt and Au metal centers

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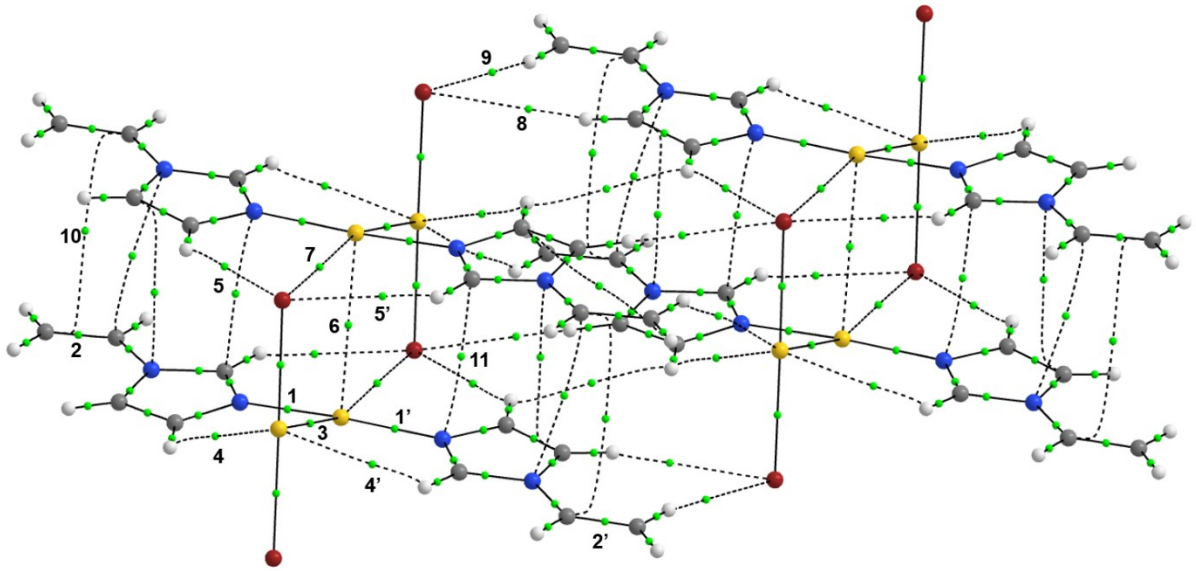


Figure S1. Bond paths and bond critical points (BCPs = small light green balls) in the extended model of the crystal structure of **2**. The numbering scheme of the BCPs is followed in Table 1.

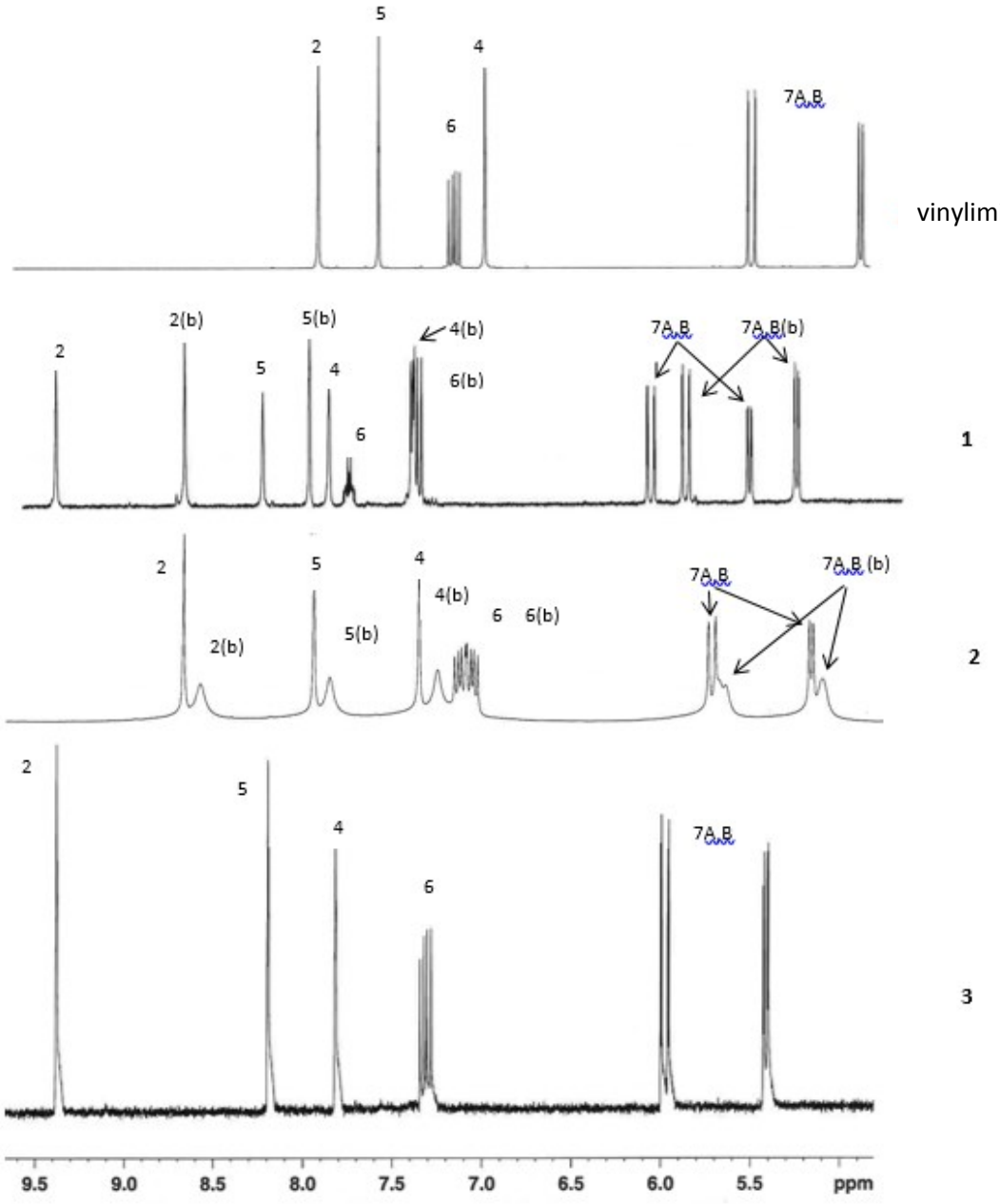
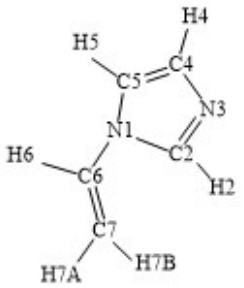
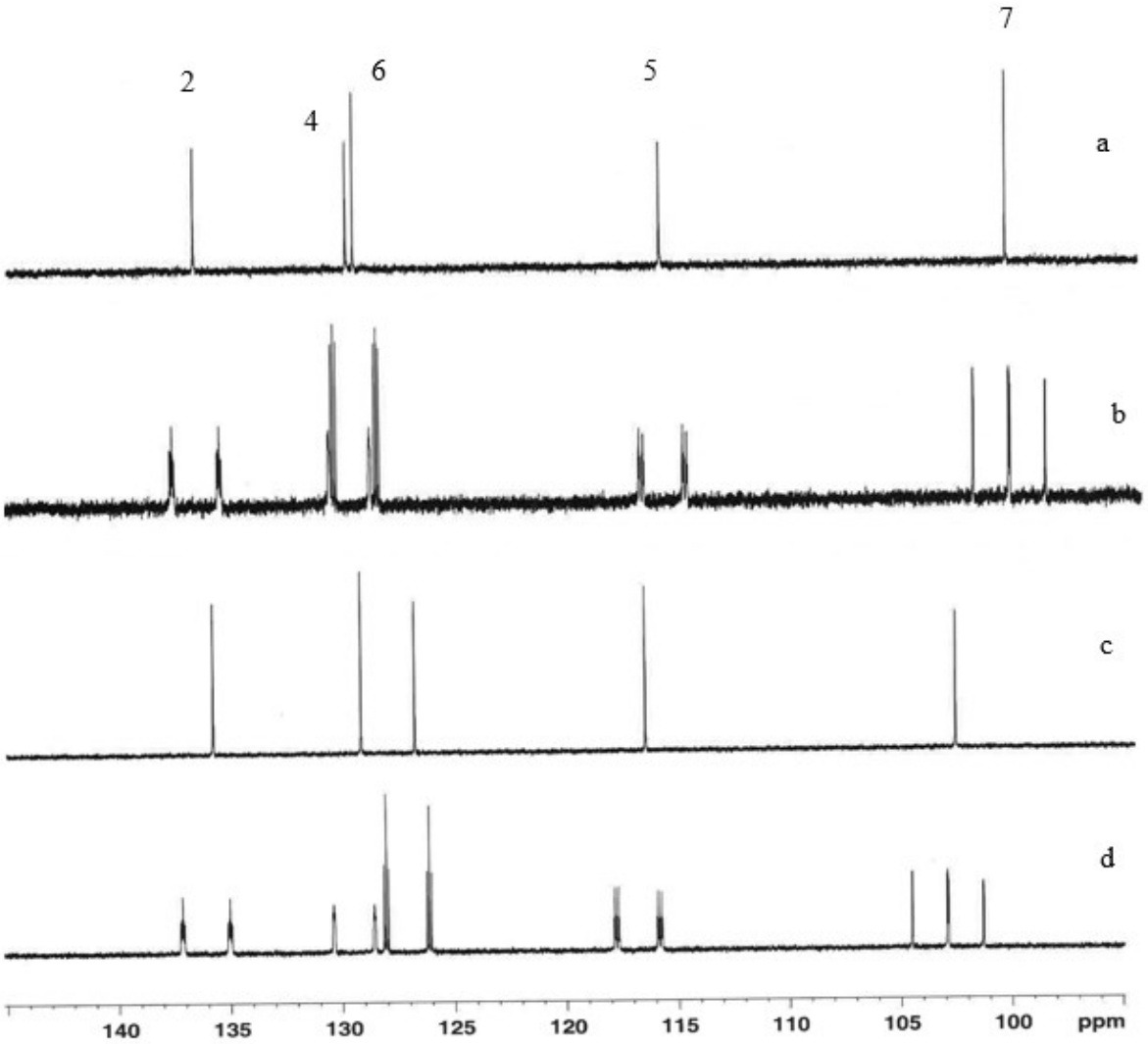


Figure S2. The ^{1}H nmr spectra of vinylimidazole and compounds **1-3** (the spectrum of **4** is similar with **3**) (Small letter b refers to the second isomer/conformer in the solution)





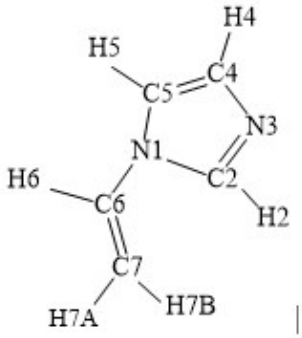
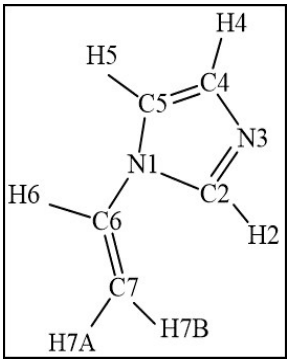


Figure S3. $^{13}C\{^{1}H\}$ and ^{13}C NMR spectra for vinylimidazole (a,b) and Hvinylimidazole (b,c)

Table S1. Experimental (d_6-DMSO) and calculated[68-70] ^{13}C spectra for vinylimidazole and compounds **1**-**4.**

Carbon / Compound	**2**	**4**	**5**	**6**	**7**
Exp. Vinylimidazole	136.6	129.9	116.1	129.6	100.8
Calc. Vinylimidazole[68-70]	136.2	130.2	115.8	129.5	101.4
Exp. Vinylimidazole+HCl	136.1	129.5	116.9	127.4	102.9
1	138.0	128.9	118.6	120.8	108.5
2	139.9	130.0	118.4	129.2	106.3
3	134.8	128.9	118.6	120.9	108.6
4	134.9	128.9	118.7	120.9	108.7



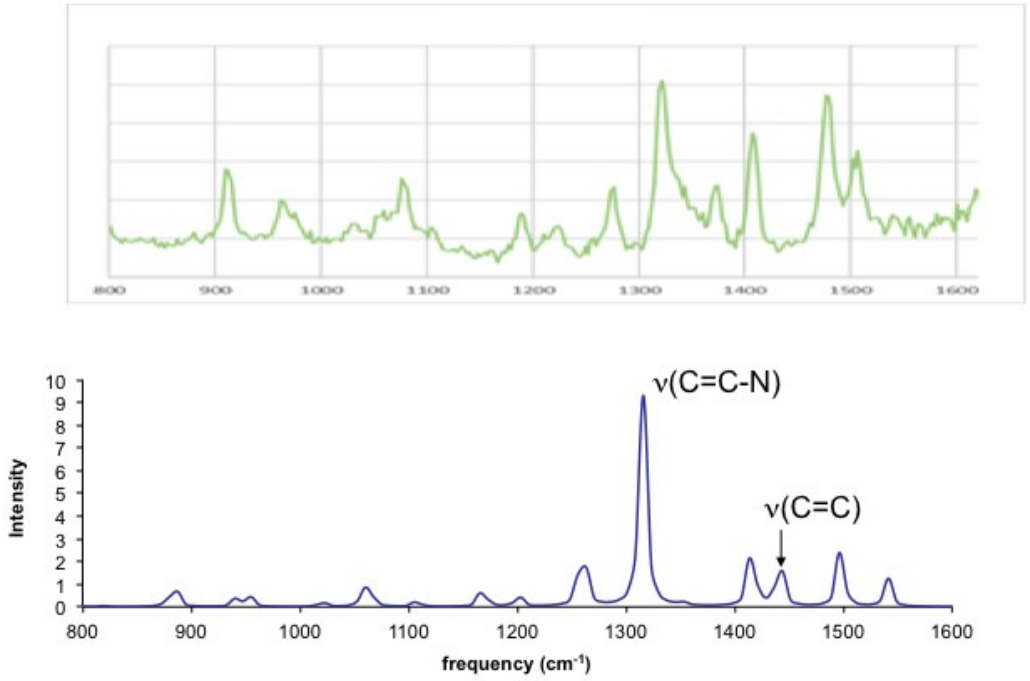


Figure S4. Experimental and simulated Raman spectrum of **1** at the region 800-1600 cm-

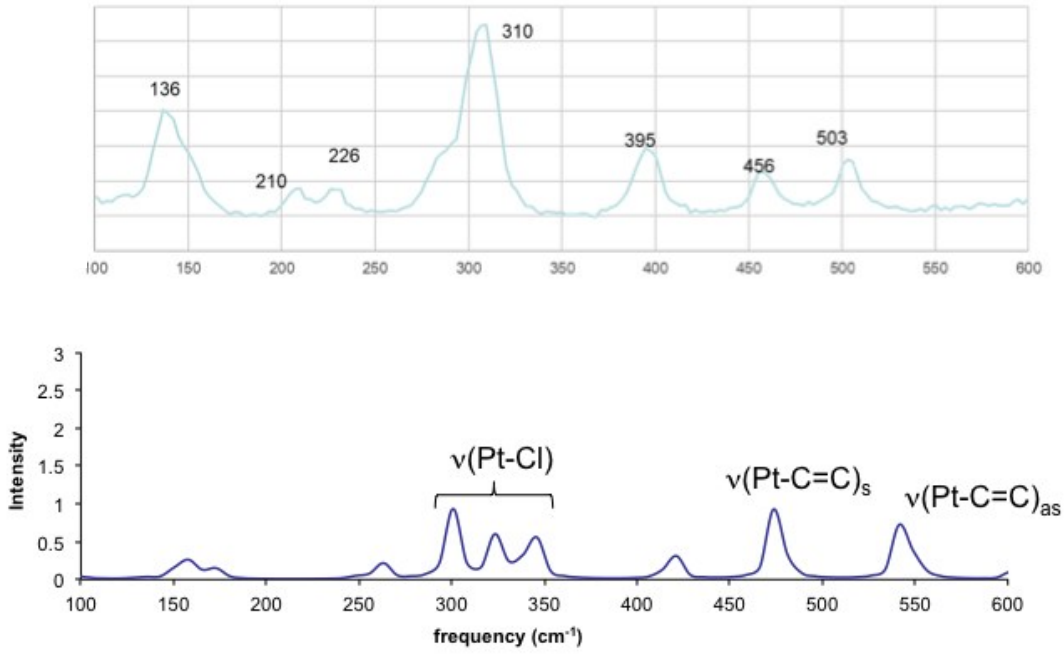
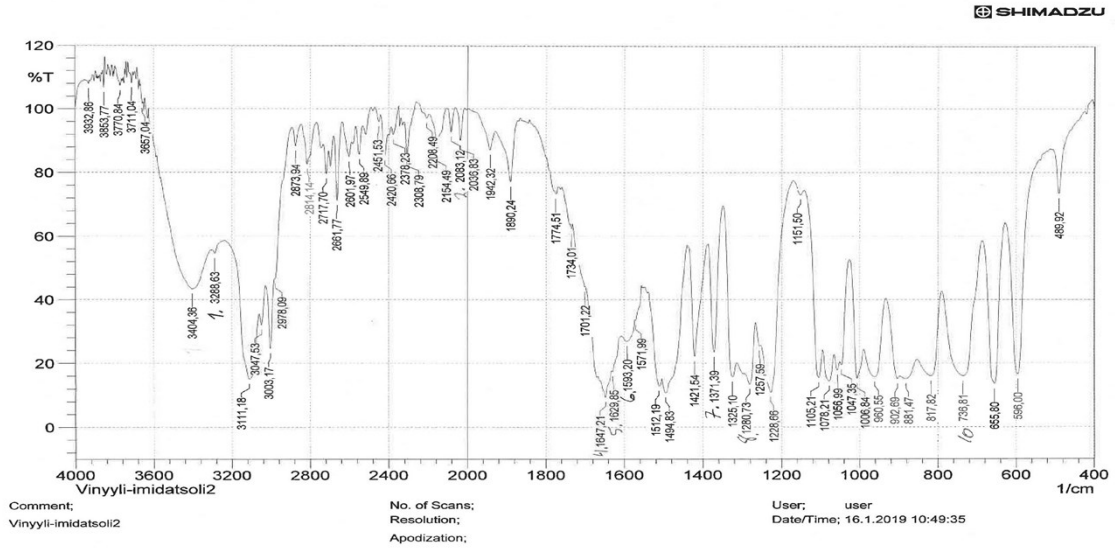


Figure S5. Experimental and simulated Raman spectrum of **1** at the region 100-600 cm-1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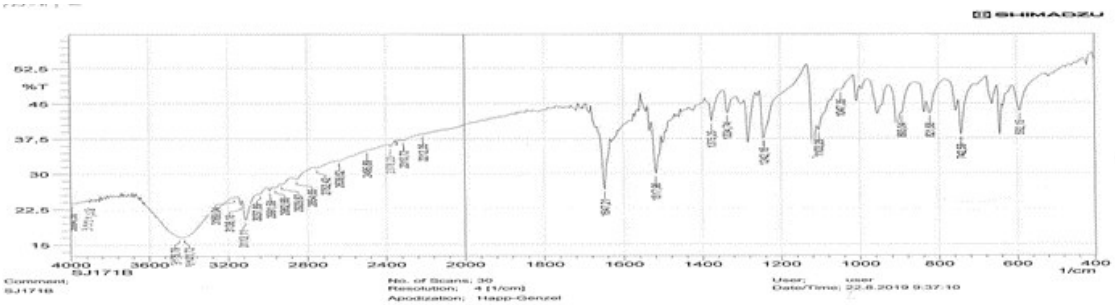
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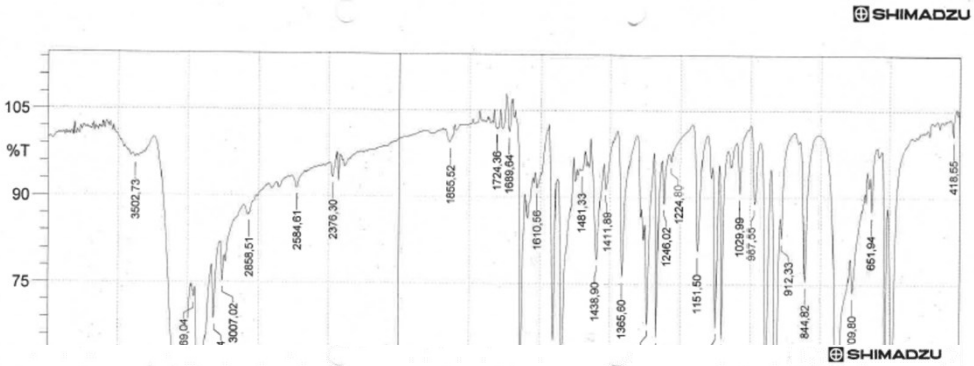
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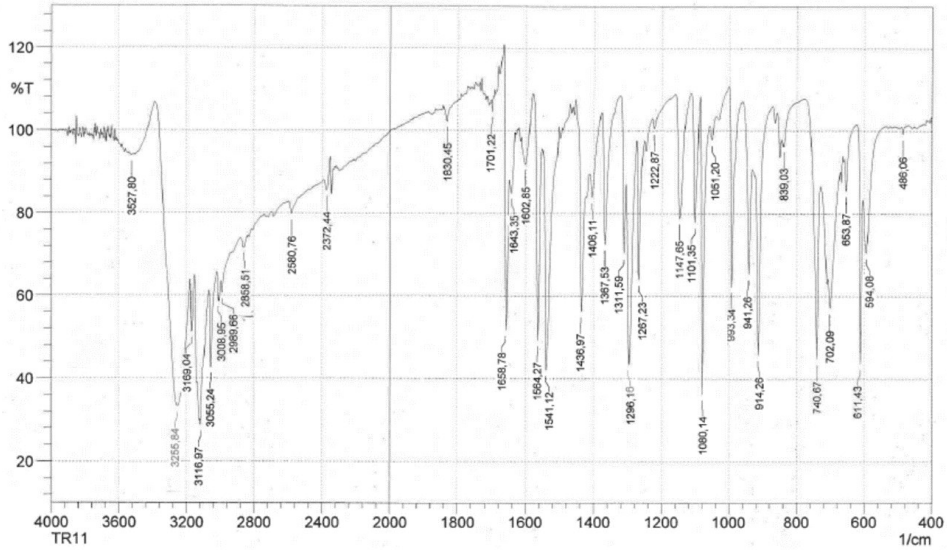
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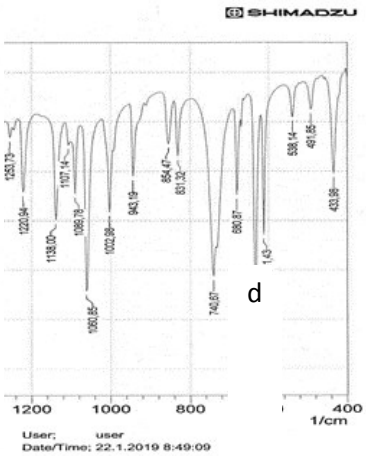
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d

e

Figure S6. Experimental IR spectrum of

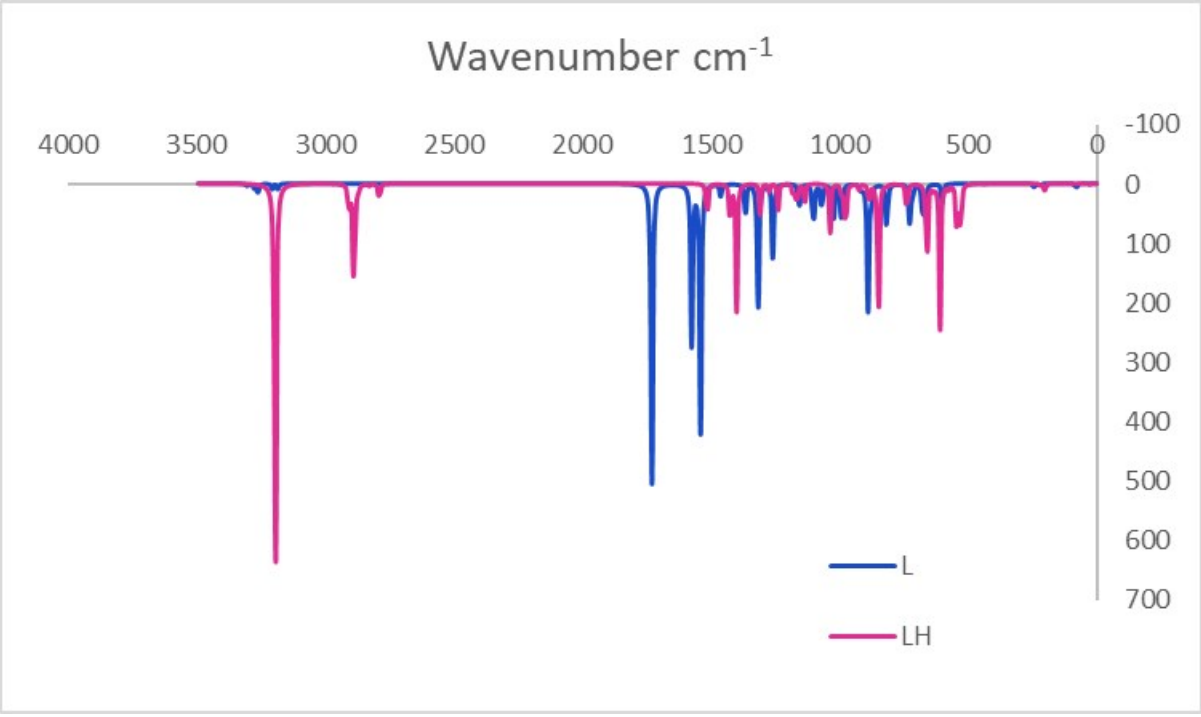
a Vinylimidazole

b $[PtCl_3(Hvinylimidazole)]$ (1) υ(N-H) 3281, υ(C=C,vinyl) 1437 cm^{-1}.

c $[Au(vinylimidazole)_2]^+[AuBr_2]^-$ (2) υ(C=C,vinyl) 1640 cm^{-1}.

d $[Hvinylimidazole]^+[AuCl_4]^-$ (3) υ(N-H) 3254, υ(C=C) 1640 cm^{-1}.

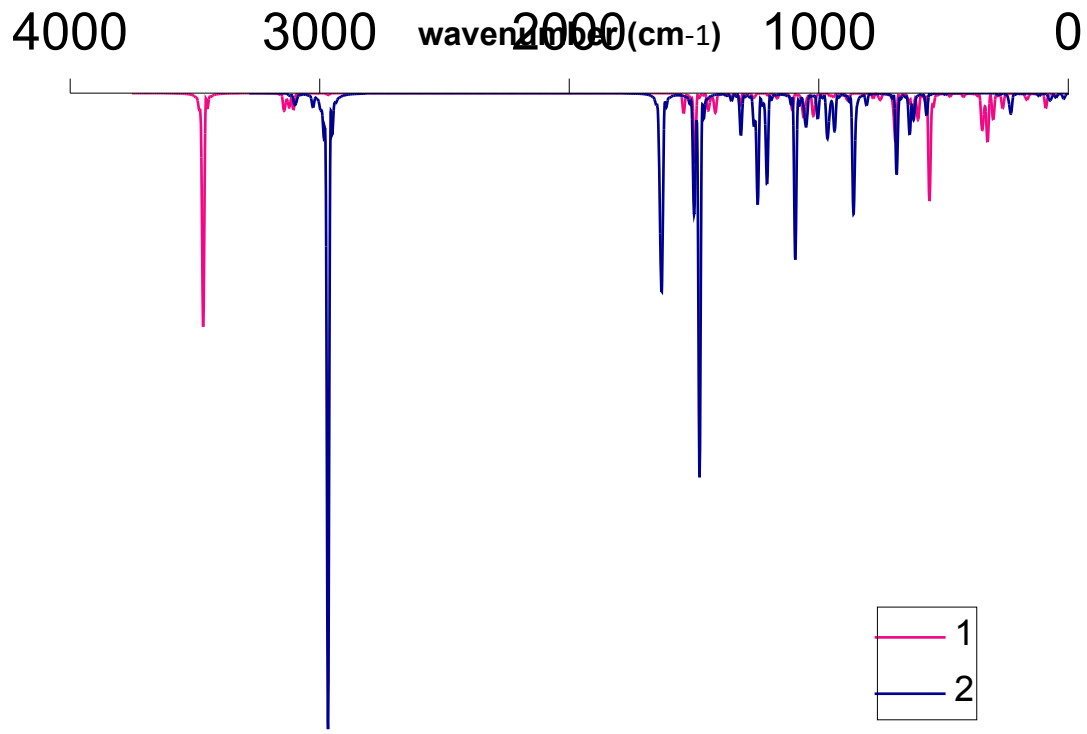
e $[Hvinylimidazole]^+[AuBr_4]^-$ (4) υ(N-H) 3256, υ(C=C) 1640 cm^{-1}.



	LH	L
ν(N-H)	3431	

νC_Hring	3102	3062
ν(C=C)vinyl	1624	1626
ν(C-H)vinyl		3080

Figure S7. Simulated IR spectrum of vinylimidazole and protonated vinylimidazole.



	1	2
ν(N-H)	3468	
νC_Hring	3141	2967
ν(C=C)vinyl	1441	1632
ν(C-H)vinyl	3055	3083

Figure S8. Simulated IR spectra of optimized structures of $[PtCl_3(Hvinylimidazole)]$ (1) and $[Au(vinylimidazole)_2]^+[AuBr_2]^-$ (2).

Table S2. Bond length and angle data for 1-4

Selected bond lengths [Å] and angles [°] for **1**

C(2)-N(3)	1.322(2)
C(2)-N(1)	1.336(2)
C(4)-C(5)	1.351(2)
C(4)-N(3)	1.371(2)
C(5)-N(1)	1.385(2)
C(6)-C(7)	1.395(2)
C(6)-N(1)	1.420(2)
C(6)-Pt(1)	2.1358(17)
C(7)-Pt(1)	2.1092(17)
Cl(1)-Pt(1)	2.3056(5)
Cl(2)-Pt(1)	2.2972(5)
Cl(3)-Pt(1)	2.2922(5)
N(3)-C(2)-N(1)	108.03(15)
C(5)-C(4)-N(3)	106.98(16)
C(4)-C(5)-N(1)	106.74(15)
C(7)-C(6)-N(1)	122.77(15)
C(7)-C(6)-Pt(1)	69.79(10)
N(1)-C(6)-Pt(1)	115.11(11)
C(6)-C(7)-Pt(1)	71.86(10)
C(2)-N(1)-C(5)	108.62(14)
C(2)-N(1)-C(6)	127.33(15)
C(5)-N(1)-C(6)	124.02(14)
C(2)-N(3)-C(4)	109.62(14)
C(7)-Pt(1)-C(6)	38.35(7)
C(7)-Pt(1)-Cl(3)	88.65(5)
C(6)-Pt(1)-Cl(3)	93.70(4)
C(7)-Pt(1)-Cl(2)	90.79(5)
C(6)-Pt(1)-Cl(2)	87.02(4)
Cl(3)-Pt(1)-Cl(2)	178.052(17)

C(7)-Pt(1)-Cl(1)	160.92(5)
C(6)-Pt(1)-Cl(1)	160.51(5)
Cl(3)-Pt(1)-Cl(1)	90.815(19)
Cl(2)-Pt(1)-Cl(1)	89.096(19)

Bond lengths [Å] and angles [°] for **2**

C(2)-N(3)	1.304(8)
C(2)-N(1)	1.360(8)
C(2A)-N(3A)	1.309(8)
C(2A)-N(1A)	1.358(8)
C(4)-C(5)	1.357(9)
C(4)-N(3)	1.373(9)
C(4A)-C(5A)	1.369(9)
C(4A)-N(3A)	1.373(8)
C(5)-N(1)	1.371(8)
C(5A)-N(1A)	1.369(9)
C(6)-C(7)	1.306(10)
C(6)-N(1)	1.415(8)
C(6A)-C(7A)	1.300(10)
C(6A)-N(1A)	1.414(8)
N(3)-Au(1)	2.017(5)
N(3A)-Au(1)	2.018(5)
Br(1)-Au(2)	2.3826(9)
Br(2)-Au(2)	2.3843(9)
Au(1)-Au(2)	3.1200(5)

N(3)-C(2)-N(1)	109.6(5)
N(3A)-C(2A)-N(1A)	110.5(6)
C(5)-C(4)-N(3)	109.3(6)
C(5A)-C(4A)-N(3A)	107.6(5)
C(4)-C(5)-N(1)	105.5(6)
N(1A)-C(5A)-C(4A)	107.4(6)
C(7)-C(6)-N(1)	125.1(7)
C(7A)-C(6A)-N(1A)	124.3(7)
C(2)-N(1)-C(5)	108.2(5)
C(2)-N(1)-C(6)	124.5(6)
C(5)-N(1)-C(6)	127.3(6)
C(2A)-N(1A)-C(5A)	106.7(5)
C(2A)-N(1A)-C(6A)	123.8(6)
C(5A)-N(1A)-C(6A)	129.4(6)
C(2)-N(3)-C(4)	107.4(5)
C(2)-N(3)-Au(1)	125.4(5)
C(4)-N(3)-Au(1)	127.1(4)

C(2A)-N(3A)-C(4A)	107.8(5)
C(2A)-N(3A)-Au(1)	126.3(5)
C(4A)-N(3A)-Au(1)	125.8(4)
N(3)-Au(1)-N(3A)	176.1(2)
N(3)-Au(1)-Au(2)	91.01(16)
N(3A)-Au(1)-Au(2)	90.82(16)
Br(1)-Au(2)-Br(2)	177.81(3)
Br(1)-Au(2)-Au(1)	93.20(2)
Br(2)-Au(2)-Au(1)	88.98(2)

Symmetry transformations used to generate equivalent atoms:

Bond lengths [Å] and angles [°] for

C(6)-C(7)	1.302(5)
C(6)-N(1)	1.427(4)
C(2)-N(3)	1.313(4)
C(2)-N(1)	1.321(4)
C(4)-C(5)	1.326(6)
C(4)-N(3)	1.379(5)
C(5)-N(1)	1.378(4)
C(6A)-C(7A)	1.257(17)
C(6A)-N(1A)	1.426(15)
C(2A)-N(1A)	1.327(8)
C(2A)-N(3A)	1.338(9)
N(1A)-C(5A)	1.358(9)
C(5A)-C(4A)	1.350(7)
C(4A)-N(3A)	1.352(10)
Cl(1)-Au(1)	2.2789(4)
Cl(4)-Au(2)	2.2798(5)
Cl(3)-Au(2)	2.2763(5)
Cl(2)-Au(1)	2.2738(5)

C(7)-C(6)-N(1)	123.8(3)
N(3)-C(2)-N(1)	108.4(3)
C(5)-C(4)-N(3)	106.3(5)
C(4)-C(5)-N(1)	107.9(5)
C(2)-N(1)-C(5)	108.1(4)
C(2)-N(1)-C(6)	124.0(3)
C(5)-N(1)-C(6)	127.8(4)
C(2)-N(3)-C(4)	109.3(5)
C(7A)-C(6A)-N(1A)	126.0(10)
N(1A)-C(2A)-N(3A)	108.4(14)
C(2A)-N(1A)-C(5A)	109.0(13)
C(2A)-N(1A)-C(6A)	123.9(10)

C(5A)-N(1A)-C(6A)	127.1(12)
C(4A)-C(5A)-N(1A)	106.2(17)
C(5A)-C(4A)-N(3A)	109(2)
C(2A)-N(3A)-C(4A)	107.3(18)
Cl(2)#1-Au(1)-Cl(1)	90.087(19)
Cl(2)-Au(1)-Cl(1)	89.913(19)
Cl(2)#1-Au(1)-Cl(1)#1	89.913(19)
Cl(2)-Au(1)-Cl(1)#1	90.087(19)
Cl(3)#2-Au(2)-Cl(4)	90.400(18)
Cl(3)-Au(2)-Cl(4)	89.600(18)
Cl(3)#2-Au(2)-Cl(4)#2	89.600(18)
Cl(3)-Au(2)-Cl(4)#2	90.400(18)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x,-y-1,-z

Bond lengths [Å] and angles [°] for **4**

C(2)-N(3)	1.311(4)
C(2)-N(1)	1.336(3)
C(4)-C(5)	1.338(4)
C(4)-N(3)	1.372(4)
C(5)-N(1)	1.382(3)
C(6)-C(7)	1.291(4)
C(6)-N(1)	1.419(3)
Br(1)-Au(1)	2.4260(2)
Br(2)-Au(1)	2.4236(2)
Br(3)-Au(2)	2.4286(2)
Br(4)-Au(2)	2.4227(2)

N(3)-C(2)-N(1)	107.8(2)
C(5)-C(4)-N(3)	106.1(2)
C(4)-C(5)-N(1)	107.6(2)
C(7)-C(6)-N(1)	124.4(3)
C(2)-N(1)-C(5)	108.1(2)
C(2)-N(1)-C(6)	124.3(2)
C(5)-N(1)-C(6)	127.6(2)
C(2)-N(3)-C(4)	110.3(2)

Br(2)-Au(1)-Br(2)#1	180.000(12)
Br(2)-Au(1)-Br(1)#1	90.260(8)
Br(2)#1-Au(1)-Br(1)#1	89.739(8)
Br(2)-Au(1)-Br(1)	89.740(8)
Br(2)#1-Au(1)-Br(1)	90.260(8)
Br(1)#1-Au(1)-Br(1)	180.0
Br(4)-Au(2)-Br(4)#2	180.0
Br(4)-Au(2)-Br(3)#2	90.289(8)
Br(4)#2-Au(2)-Br(3)#2	89.711(8)
Br(4)-Au(2)-Br(3)	89.711(8)
Br(4)#2-Au(2)-Br(3)	90.288(8)
Br(3)#2-Au(2)-Br(3)	180.0

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