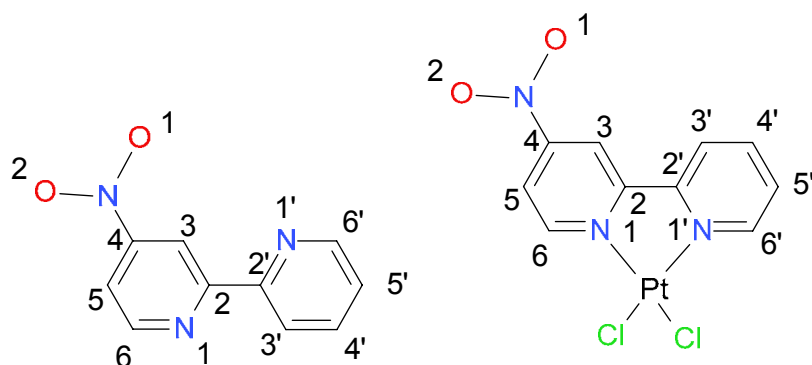


## Determining the Site of Reduction of 4-NO<sub>2</sub>-2,2'-bipyridine and [Pt(4-NO<sub>2</sub>-2,2'-bipyridine)Cl<sub>2</sub>]

Paul Murray,<sup>\*a</sup> Lorna Jack,<sup>a</sup> Eric J. L. McInnes<sup>b</sup> and Lesley J. Yellowlees<sup>a</sup>



### Calculated Bond Lengths

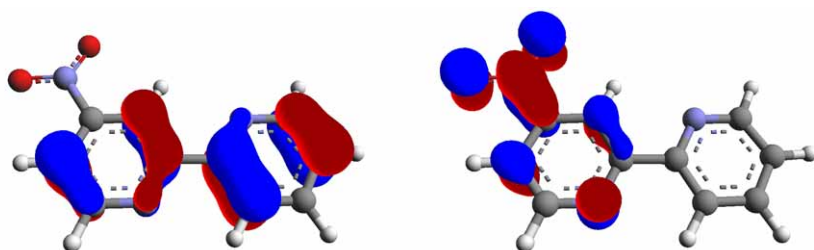
	4-NO <sub>2</sub> -bpy /Å	[4-NO <sub>2</sub> -bpy] <sup>1-</sup> /Å	[Pt(4-NO <sub>2</sub> -bpy)] /Å	[Pt(4-NO <sub>2</sub> -bpy)] <sup>1-</sup> /Å	[Pt(4-NO <sub>2</sub> -bpy)] <sup>2-</sup> /Å
N1-C2	1.3	1.4	1.4	1.4	1.4
C2-C3	1.4	1.4	1.4	1.4	1.4
C3-C4	1.4	1.4	1.4	1.4	1.4
C4-C5	1.4	1.4	1.5	1.4	1.5
C5-C6	1.4	1.4	1.4	1.4	1.4
C6-N1	1.3	1.3	1.4	1.4	1.4
C3-H3	1.1	1.1	1.1	1.1	1.1
C4-N4	1.5	1.4	1.4	1.4	1.4
N4-O1	1.2	1.3	1.3	1.3	1.3
N4-O2	1.2	1.3	1.3	1.3	1.3
C5-H5	1.1	1.1	1.1	1.1	1.1
C6-H6	1.1	1.1	1.1	1.1	1.1
C2-C2'	1.4	1.5	1.4	1.5	1.4
N1'-C2'	1.3	1.4	1.4	1.4	1.4
C2'-C3'	1.4	1.4	1.4	1.4	1.4
C3'-C4'	1.4	1.4	1.4	1.4	1.4
C4'-C5'	1.4	1.4	1.4	1.4	1.4
C5'-C6'	1.4	1.4	1.4	1.4	1.4
C6'-N1'	1.3	1.3	1.3	1.3	1.3
C3'-H3'	1.1	1.1	1.1	1.1	1.1
C4'-H4'	1.1	1.1	1.1	1.1	1.1
C5'-H5'	1.1	1.1	1.1	1.1	1.1
C6'-H6'	1.1	1.1	1.1	1.1	1.1
Pt-N1	-	-	2.0	2.0	2.0
Pt-N1'	-	-	2.0	2.0	2.0
Pt-Cl1	-	-	2.4	2.4	2.4
Pt-Cl2	-	-	2.4	2.4	2.4

**Calculated Bond Angles**

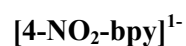
	4-NO <sub>2</sub> -bpy /°	[4-NO <sub>2</sub> -bpy] <sup>1-</sup> /°	[Pt(4-NO <sub>2</sub> -bpy)] /°	[Pt(4-NO <sub>2</sub> -bpy)] <sup>1-</sup> /°	[Pt(4-NO <sub>2</sub> -bpy)] <sup>2-</sup> /°
N1-C2-C3	122.3	123.6	120.9	121.4	121.0
C2-C3-C4	117.3	119.1	118.2	119.8	121.1
C3-C4-C5	121.6	117.8	121.2	118.6	117.4
C4-C5-C6	116.4	118.0	117.6	118.7	118.6
C5-C6-N1	123.8	125.4	122.1	123.1	124.2
C6-N1-C2	118.8	116.1	120.0	118.5	117.7
N1-C2-C2'	117.4	115.9	114.9	114.7	115.3
C3-C2-C2'	120.3	120.6	124.2	123.8	123.7
C2-C3-H3	120.7	121.0	122.3	122.1	121.1
H3-C3-C4	122.0	119.9	119.4	118.2	117.7
C3-C4-N4	119.3	121.1	119.0	119.9	120.2
N4-C4-C5	119.1	121.1	119.8	121.5	122.4
C4-N4-O1	117.7	118.4	117.2	118.8	120.5
C4-N4-O2	117.3	119.3	117.1	118.1	118.5
O1-N4-O2	125.0	122.3	125.6	123.1	121.0
C4-C5-H5	121.3	119.8	121.2	120.1	120.0
H5-C5-C6	122.3	122.2	121.2	121.2	121.4
C5-C6-H6	120.1	119.3	123.1	122.3	121.6
H6-C6-N1	116.2	115.4	114.9	114.6	114.2
N1'-C2'-C3'	122.6	121.2	121.0	120.0	118.9
C2'-C3'-C4'	118.6	119.4	119.4	120.0	121.0
C3'-C4'-C5'	119.0	119.2	118.9	119.0	118.9
C4'-C5'-C6'	118.2	117.5	119.3	118.9	118.4
C5'-C6'-N1'	123.4	117.5	121.7	122.2	123.1
C6'-N1'-C2'	118.2	118.6	119.8	119.9	119.6
N1'-C2'-C2	116.5	118.6	114.6	115.0	114.8
C3'-C2'-C2	120.9	120.2	124.5	125.0	126.2
C2'-C3'-H3'	119.5	118.3	120.4	119.5	118.7
H3'-C3'-C4'	121.9	122.4	120.2	120.5	120.4
C3'-C4'-H4'	120.3	120.3	120.2	120.1	120.2
H4'-C4'-C5'	120.7	120.6	120.9	120.8	120.9
C4'-C5'-H5'	121.5	121.9	121.5	121.7	122.0
H5'-C5'-C6'	120.3	120.7	119.2	119.4	119.6
C5'-C6'-H6'	120.6	120.2	123.4	123.3	122.6
H6'-C6'-N1'	116.0	115.8	114.0	114.6	114.3
C2-N1-Pt	-	-	115.2	114.8	114.3
C6-N1-Pt	-	-	124.9	126.7	128.0
C2'-N1'-Pt	-	-	115.0	115.1	114.8
C6'-N1'-Pt	-	-	125.2	125.0	125.6
N1-Pt-N1'	-	-	94.9	80.4	80.7
N1-Pt-Cl1	-	-	89.9	95.1	95.4
Cl-Pt-Cl'	-	-	89.8	89.7	89.1
N1'-Pt-Cl'	-	-	94.9	94.7	94.7

**Calculated Energies and Molecular Orbitals**4-NO<sub>2</sub>-bpy

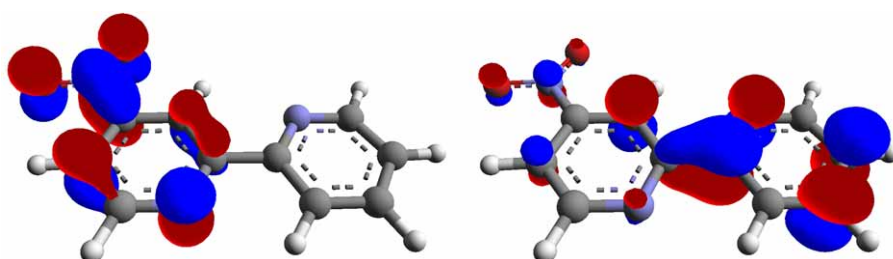
Total energy = -699.9225357 Hartrees



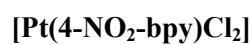
HOMO (left) and LUMO (right) of 4-NO<sub>2</sub>-bpy, energies = -0.26460 and -0.11874 Hartrees respectively



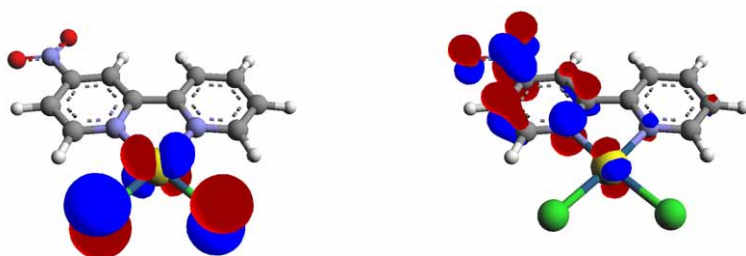
Total energy = -699.985228 Hartrees



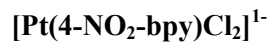
SOMO (left) and LUMO (right) of [4-NO<sub>2</sub>-bpy]<sup>1-</sup>, energies = -0.00796 and 0.05240 Hartrees respectively



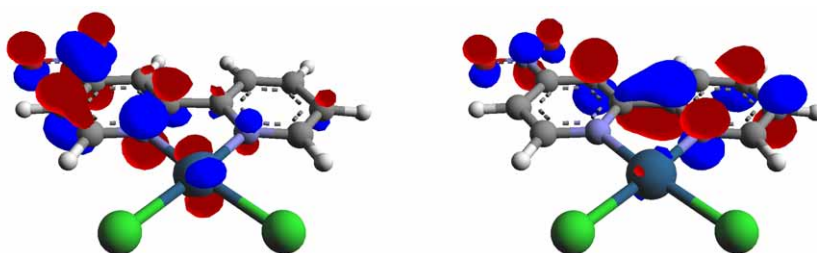
Total energy = -1739.2490721 Hartrees



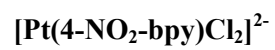
HOMO (left) and LUMO (right) of [Pt(4-NO<sub>2</sub>-bpy)Cl<sub>2</sub>], energies = -0.24124 and -0.15411 Hartrees respectively



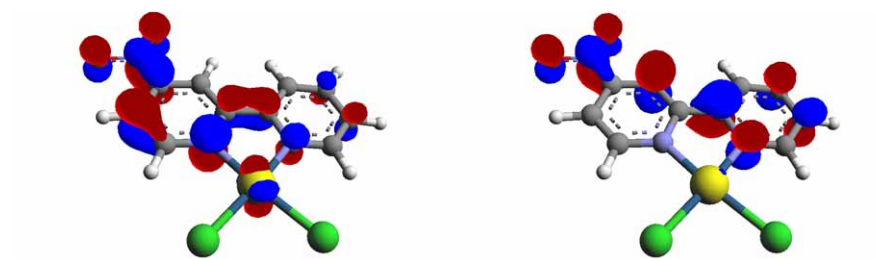
Total energy = -1739.3540944 Hartrees



SOMO (left) and LUMO (right) of [Pt(4-NO<sub>2</sub>-bpy)Cl<sub>2</sub>]<sup>1-</sup>, energies = -0.05633 and 0.00253 Hartrees respectively



Total energy = -1739.3080975 Hartrees



**HOMO (left) and LUMO (right) of [Pt(4-NO<sub>2</sub>-bpy)Cl<sub>2</sub>]<sup>2-</sup>, energies = 0.09085 and 0.13882 Hartrees respectively**