Supplementary Material for the paper to Dalton Trans:

Synthesis, characterization, DNA binding properties and electronic structure (DFT) of the new complex *cis*-(*Cl,Cl*)[$Ru^{II}Cl_2(NO^+)$(terpy)]Cl.

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Table S1. Selected bond lengths (pm), bond angles (°), and uscaled *v*(N-O) harmonic vibrational frequencies (cm^{-1}) of the *cis*- and *trans*-(*Cl,Cl*)-$[Ru(terpy)(NO)Cl_2]^+$ complexes calculated at the B3LYP level and comparison with available experimental data.

Parameter	*cis*-(*Cl,Cl*)-$[Ru(terpy)(NO)Cl_2]^+$			*trans*-(*Cl,Cl*)-$[Ru(terpy)(NO)Cl_2]^+$			
	SDD	6-31G(d)[a]	DZVP[b]	SDD	6-31G(d)	DZVP	expt.[c]
R_e(Ru-N1)	176.4	179.0	179.3	175.8	178.0	178.2	176.5
R_e(N1-O)	119.0	114.8	115.0	118.8	114.8	114.9	112.9
R_e(Ru-Cl1)	244.2	242.4	242.4	243.1	241.0	241.5	237.5
R_e(Ru-Cl2)	238.8	234.8	235.8	243.1	241.0	241.5	235.3
R_e(Ru-N2)	210.0	212.4	213.6	209.6	212.2	212.9	208.3
R_e(Ru-N3)	201.4	203.4	204.2	203.7	205.0	205.6	201.5
R_e(Ru-N4)	210.0	212.4	213.6	209.6	212.3	212.9	207.3
∠Ru-N1-O	173.6	170.3	173.0	180.0	180.0	180.0	174.6
∠N1-Ru-Cl1	86.8	84.4	85.9	94.8	95.2	94.8	
∠N1-Ru-Cl2	175.0	173.1	174.6	94.8	95.3	94.8	
∠Cl1-Ru-Cl2	88.1	88.7	88.7	170.5	169.5	170.3	
∠N1-Ru-N2	95.3	95.1	95.0	101.7	102.2	102.3	
∠N3-Ru-N4	158.4	157.5	156.9	156.7	155.6	155.3	157.4
∠O-N1-Ru-Cl1	0.2	0.0	0.2	15.1	0.0	12.0	
v(N-O)	1812 1860[d]	1985	1968	1829	1993	1987	1895

[a] The LANL2DZ basis set was used for ruthenium combined with the 6-31G(d) basis set for all non metal atoms. [b] The SDD basis set was used for ruthenium combined with the DZVP basis set for all non metal atoms. [b] Experimental structural parameters taken from Ref. 28. [d] Experimental value taken from this work.

Table S2. GIAO-B3LYP/SDD ^{13}C, ^{15}N, ^{17}O and ^{1}H NMR absolute isotropic shielding tensor elements (σ, ppm) of the *cis*- and *trans*-(*Cl,Cl*)-[Ru(terpy)(NO)Cl_2]$^+$ Complexes Computed at the B3LYP/SDD level.

***cis*-(*Cl,Cl*)-[Ru(terpy)(NO)Cl_2]$^+$**

SCF GIAO Magnetic shielding tensor (ppm):

1	N	Isotropic =	-16.1558	Anisotropy =	372.6596
2	C	Isotropic =	30.3089	Anisotropy =	135.6726
3	C	Isotropic =	63.9317	Anisotropy =	184.9129
4	C	Isotropic =	47.8608	Anisotropy =	215.0835
5	C	Isotropic =	58.6901	Anisotropy =	187.8139
6	C	Isotropic =	31.9017	Anisotropy =	187.7966
7	N	Isotropic =	-20.5905	Anisotropy =	329.9345
8	C	Isotropic =	32.9865	Anisotropy =	151.7136
9	C	Isotropic =	66.0283	Anisotropy =	180.7730
10	C	Isotropic =	46.1236	Anisotropy =	210.9658
11	C	Isotropic =	66.0279	Anisotropy =	180.7724
12	C	Isotropic =	32.9865	Anisotropy =	151.7167
13	Ru	Isotropic =	-657.3406	Anisotropy =	41.4165
14	N	Isotropic =	-118.0934	Anisotropy =	748.6857
15	Cl	Isotropic =	578.2876	Anisotropy =	597.7884
16	Cl	Isotropic =	947.7901	Anisotropy =	160.8675
17	N	Isotropic =	-16.1565	Anisotropy =	372.6630
18	C	Isotropic =	30.3093	Anisotropy =	135.6713
19	C	Isotropic =	63.9318	Anisotropy =	184.9120
20	C	Isotropic =	47.8601	Anisotropy =	215.0842
21	C	Isotropic =	58.6914	Anisotropy =	187.8119
22	C	Isotropic =	31.9033	Anisotropy =	187.8045
23	O	Isotropic =	-119.8035	Anisotropy =	914.7898
24	H	Isotropic =	24.0435	Anisotropy =	7.3812
25	H	Isotropic =	23.7826	Anisotropy =	4.2996
26	H	Isotropic =	24.2131	Anisotropy =	3.8700
27	H	Isotropic =	22.2944	Anisotropy =	10.5617
28	H	Isotropic =	24.1549	Anisotropy =	6.5401
29	H	Isotropic =	23.8765	Anisotropy =	4.5450
30	H	Isotropic =	24.1549	Anisotropy =	6.5400
31	H	Isotropic =	24.0436	Anisotropy =	7.3811
32	H	Isotropic =	23.7827	Anisotropy =	4.2996
33	H	Isotropic =	24.2132	Anisotropy =	3.8700
34	H	Isotropic =	22.2941	Anisotropy =	10.5629

***trans*-(*Cl,Cl*)-[Ru(terpy)(NO)Cl_2]$^+$**

SCF GIAO Magnetic shielding tensor (ppm):

1	N	Isotropic =	-26.9677	Anisotropy =	359.2997
2	C	Isotropic =	31.1011	Anisotropy =	138.5117
3	C	Isotropic =	63.9269	Anisotropy =	185.3766
4	C	Isotropic =	48.4338	Anisotropy =	215.4570
5	C	Isotropic =	58.9785	Anisotropy =	185.2230
6	C	Isotropic =	34.5604	Anisotropy =	164.9983
7	N	Isotropic =	-39.4368	Anisotropy =	320.6566
8	C	Isotropic =	32.7893	Anisotropy =	148.1028
9	C	Isotropic =	66.8734	Anisotropy =	179.3936
10	C	Isotropic =	46.2365	Anisotropy =	211.4264
11	C	Isotropic =	66.8733	Anisotropy =	179.3943
12	C	Isotropic =	32.7897	Anisotropy =	148.1051
13	Ru	Isotropic =	-695.2652	Anisotropy =	91.2730
14	Cl	Isotropic =	883.3308	Anisotropy =	351.1076
15	Cl	Isotropic =	883.1118	Anisotropy =	351.2052
16	N	Isotropic =	-196.3496	Anisotropy =	595.8527
17	O	Isotropic =	-234.1679	Anisotropy =	682.3348
18	N	Isotropic =	-26.9649	Anisotropy =	359.3045
19	C	Isotropic =	31.0996	Anisotropy =	138.5094
20	C	Isotropic =	63.9266	Anisotropy =	185.3766
21	C	Isotropic =	48.4342	Anisotropy =	215.4571
22	C	Isotropic =	58.9788	Anisotropy =	185.2235
23	C	Isotropic =	34.5627	Anisotropy =	165.0081
24	H	Isotropic =	24.1404	Anisotropy =	7.3686
25	H	Isotropic =	23.8674	Anisotropy =	4.0682

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26  H    Isotropic =    24.3264   Anisotropy =     3.4351
27  H    Isotropic =    23.4553   Anisotropy =     7.1986
28  H    Isotropic =    24.3632   Anisotropy =     6.3535
29  H    Isotropic =    24.0837   Anisotropy =     4.2535
30  H    Isotropic =    24.3631   Anisotropy =     6.3536
31  H    Isotropic =    24.1404   Anisotropy =     7.3685
32  H    Isotropic =    23.8673   Anisotropy =     4.0681
33  H    Isotropic =    24.3263   Anisotropy =     3.4352
34  H    Isotropic =    23.4554   Anisotropy =     7.1993
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Table S3. GIAO-B3LYP/SDD ^{13}C, ^{15}N, ^{17}O and ^{1}H NMR absolute isotropic shielding tensor elements (σ, ppm) of TMS, nitromethane and formamide compounds computed at the B3LYP/SDD level.

TMS

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SCF GIAO Magnetic shielding tensor (ppm):
1  Si   Isotropic =   424.6152   Anisotropy =     0.8030
2  C    Isotropic =   191.7803   Anisotropy =     7.4937
3  C    Isotropic =   191.7697   Anisotropy =     7.5833
4  C    Isotropic =   191.6718   Anisotropy =     7.6898
5  C    Isotropic =   191.7005   Anisotropy =     7.6886
6  H    Isotropic =    32.7783   Anisotropy =     9.8733
7  H    Isotropic =    32.7714   Anisotropy =     9.9135
8  H    Isotropic =    32.7720   Anisotropy =     9.9116
9  H    Isotropic =    32.7733   Anisotropy =     9.8982
10  H    Isotropic =    32.7785   Anisotropy =     9.8866
11  H    Isotropic =    32.7667   Anisotropy =     9.9185
12  H    Isotropic =    32.7825   Anisotropy =     9.8776
13  H    Isotropic =    32.7715   Anisotropy =     9.8803
14  H    Isotropic =    32.7716   Anisotropy =     9.8993
15  H    Isotropic =    32.7693   Anisotropy =     9.9075
16  H    Isotropic =    32.7736   Anisotropy =     9.8911
17  H    Isotropic =    32.7829   Anisotropy =     9.8814
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Nitromethane

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SCF GIAO Magnetic shielding tensor (ppm):
1  C    Isotropic =   120.7934   Anisotropy =   103.2583
2  N    Isotropic =  -197.9379   Anisotropy =   364.3157
3  O    Isotropic =  -559.8674   Anisotropy =   923.2106
4  O    Isotropic =  -586.3771   Anisotropy =   930.7926
5  H    Isotropic =    28.1851   Anisotropy =     3.3473
6  H    Isotropic =    28.1761   Anisotropy =     3.4547
7  H    Isotropic =    28.1986   Anisotropy =     2.9780
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Formamide

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SCF GIAO Magnetic shielding tensor (ppm):
1  C    Isotropic =    29.2138   Anisotropy =   120.6224
2  O    Isotropic =  -153.1073   Anisotropy =   727.5133
3  N    Isotropic =   144.2774   Anisotropy =   132.0867

4  H    Isotropic =    24.0641   Anisotropy =     3.7953
5  H    Isotropic =    28.0107   Anisotropy =     7.8874
6  H    Isotropic =    28.0949   Anisotropy =    10.8388
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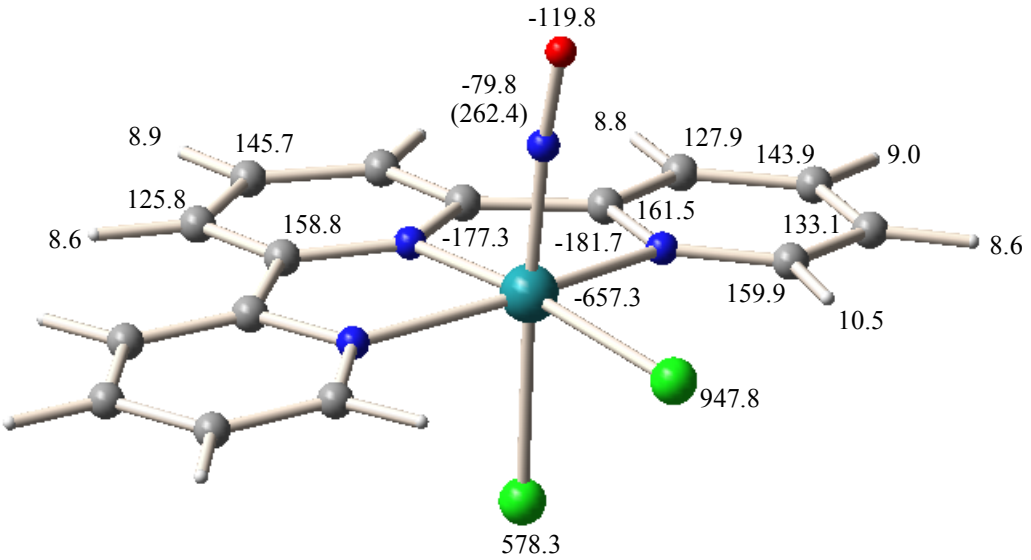

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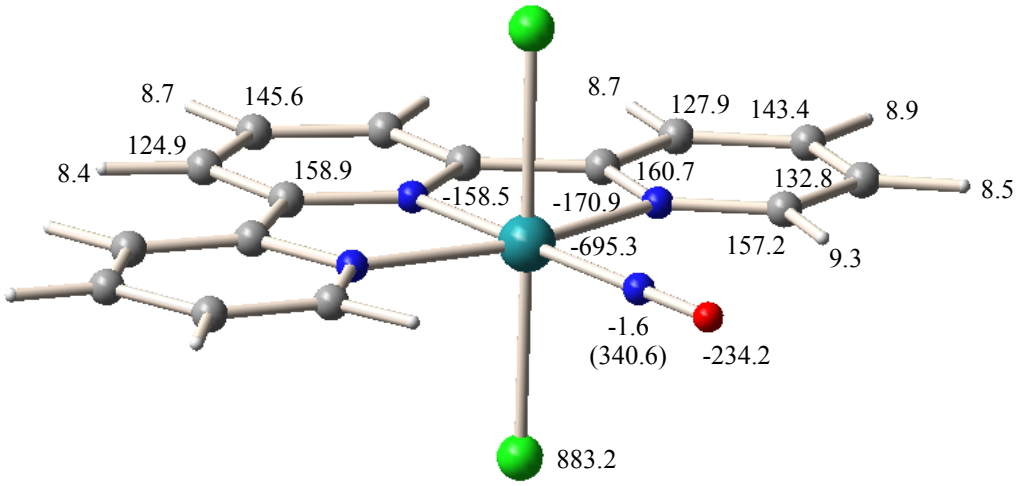

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Scheme S2: The ^{13}C, ^{15}N and ^{1}H chemical shifts for cis- and trans-dichloro(nitrosyl)(terpyridine)ruthenium(II) cation