Supplementary Information

Valence and spin situations in isomeric $[(bpy)Ru(Q^{/})_2]^n$ ($Q^{/}$ = 3,5-di-*tert*-butyl-*N*-aryl-1,2-benzoquinonemonoimine). An experimental and DFT analysis

Dipanwita Das,[a] Tapan Kumar Mondal,[b] Abhishek Dutta Chowdhury,[a] Fritz Weisser,[c] David Schweinfurth,[c] Biprajit Sarkar,[c] Shaikh M. Mobin,[a] Francisco A. Urbanos,[d] Reyes Jiménez-Aparicio,*[d] and Goutam Kumar Lahiri*[a]

[a]*Department of Chemistry, Indian Institute of Technology Bombay, Powai, Mumbai-400076, India. E-mail: lahiri@chem.iitb.ac.in*

[b]*Department of Chemistry, Jadavpur University, Jadavpur, Kolkata-700032, India*

[c]*Institut für Anorganische Chemie, Universität Stuttgart, Pfaffenwaldring 55, D-70550 Stuttgart, Germany*

[d]*Departamento de Química Inorgánica, Facultad de Ciencias Químicas, Universidad Complutense, Ciudad Universitaria, E-28040 Madrid, Spain*

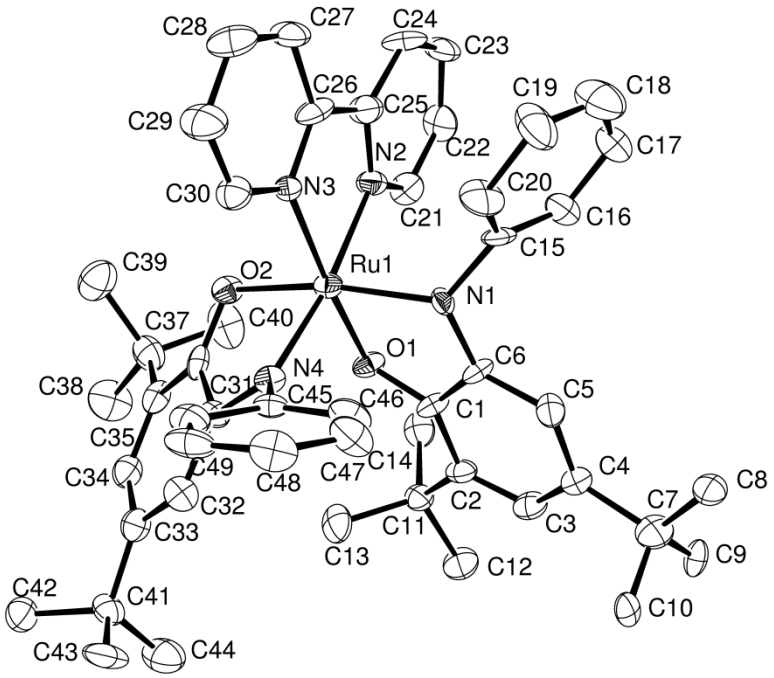


Fig. S1 ORTEP diagram of **1**. One of the independent molecules in the asymmetric Unit is shown. Ellipsoids are drawn at 35% probability.

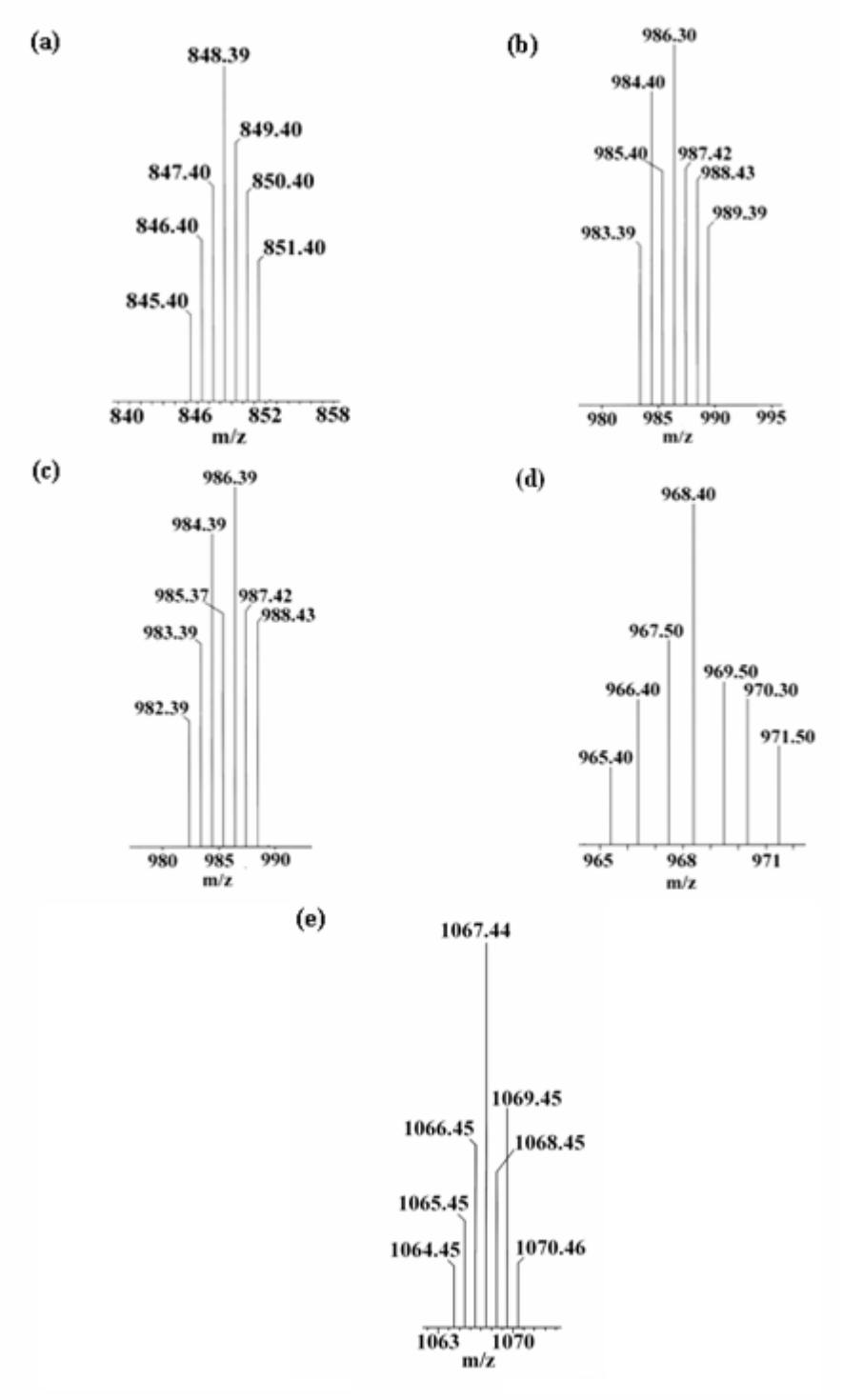


Fig. S2 ESI mass spectra of (a) **1**, (b) **2a**, (c) **2b**, (d) **3**, (e) [**3**]$(ClO_4)_2$ in CH_3CN.

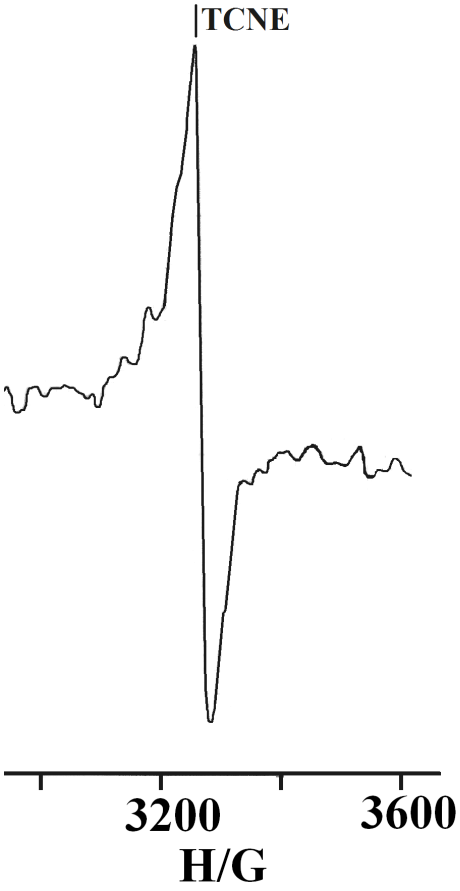


Fig. S3 EPR spectrum of **1** at 300 K in solid state.

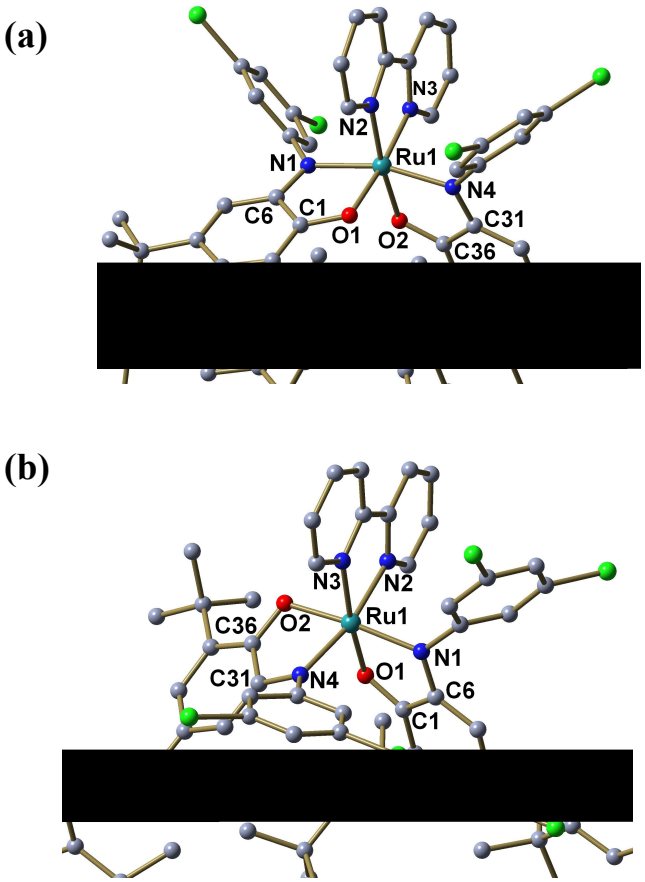


Fig. S4 DFT optimised structures of (a) **2a** and (b) **2b** in triplet (S=1) state.

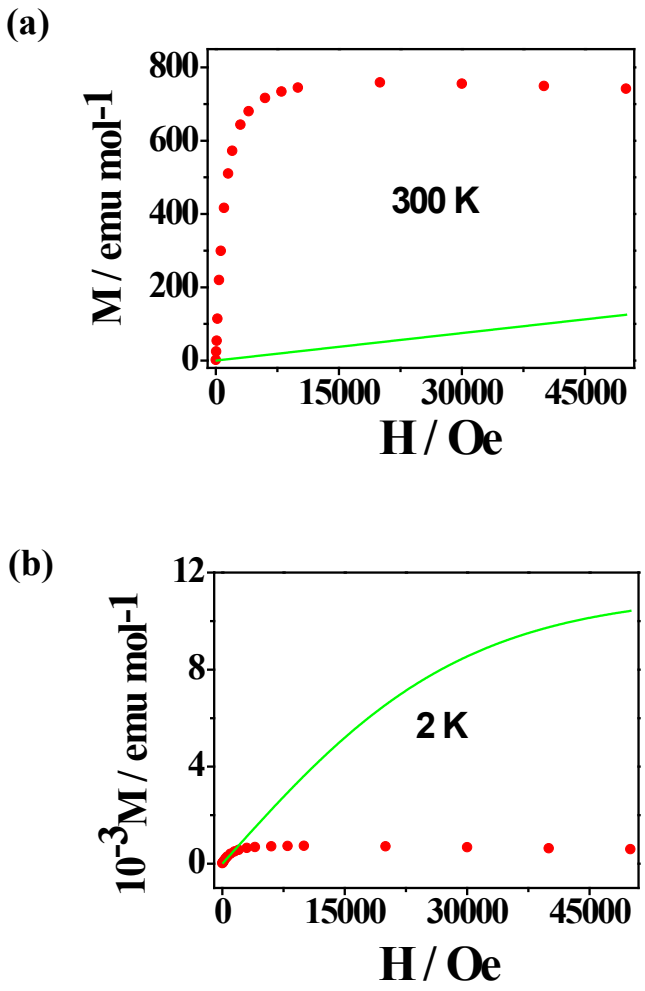


Fig. S5 Representation of the magnetization towards magnetic field from 0 to 5 T of **1** measured at (a) 300 K and (b) 2 K. Solid line represents the calculated curve for a system with two S = 1/2 spins.

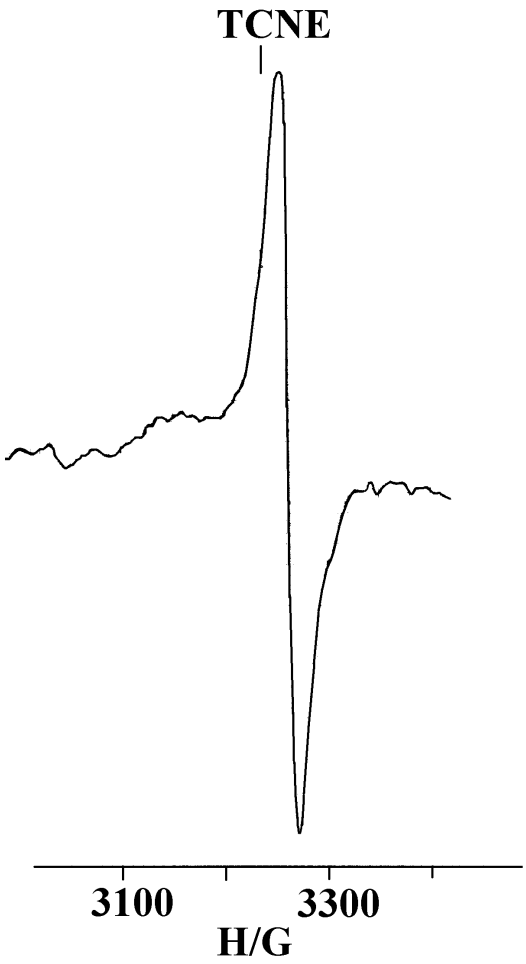


Fig. S6 EPR spectrum of $\mathbf{1}^{+}$ at 110 K in CH_3CN.

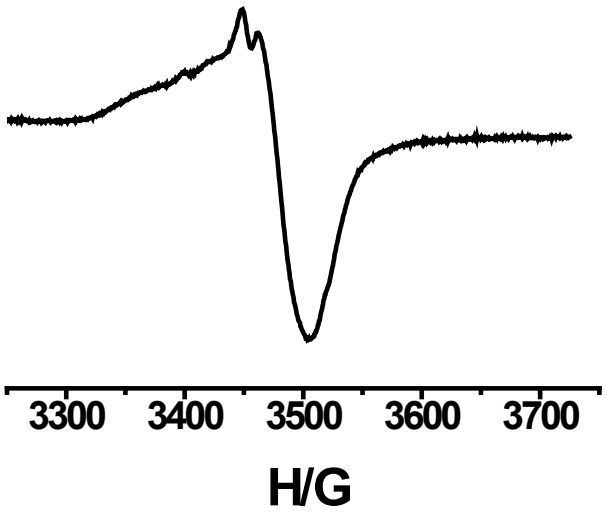


Fig. S7 EPR spectrum of **2b**$^{-}$ at 110 K in CH_3CN.

Table S1 Selected crystallographic data for **1**

	1
Empirical formula	$C_{50}H_{58}N_4O_2Ru$
M_r	848.07
Crystal symmetry	Triclinic
Space group	*P -1*
a/Å	10.306(2)
b/ Å	18.642(2)
c/ Å	24.882(2)
α /°	69.662(10)
β /°	81.914(12)
γ /°	83.063(13)
V / Å^3	4424.7(11)
Z	4
μ/mm^{-1}	0.397
T/K	150(2)
D_c/g cm^{-3}	1.273
F (000)	1784
2θ range(deg)	3.35 to 25.00
Data,restraints, parameters	15516 / 0 / 1021
Final R1, wR2 *[*I > 2σ(I)*]*	0.1665, 0.3908
R1, wR2(all data)	0.1833, 0.3969
GOF	1.123
largest diff. peak/hole, (e Å^{-3})	2.916 and -2.280

Table S2 Selected bond distances (Å) and angles (°) in **1**

Bond distances		Bond angles	
Ru(1)-N(1)	1.971(12)	N(1)-Ru(1)-N(4)	100.7(5)
Ru(1)-N(4)	1.975(12)	N(1)-Ru(1)-O(2)	163.6(3)
Ru(1)-O(2)	2.019(18)	N(4)-Ru(1)-O(2)	80.3(3)
Ru(1)-O(1)	2.000(15)	N(1)-Ru(1)-O(1)	80.2(3)
Ru(1)-N(3)	2.094(12)	N(4)-Ru(1)-O(1)	87.6(4)
Ru(1)-N(2)	2.077(13)	O(2)-Ru(1)-O(1)	83.6(6)
N(1)-C(6)	1.393(17)	N(1)-Ru(1)-N(3)	99.4(5)
O(1)-C(1)	1.310(18)	N(4)-Ru(1)-N(3)	97.8(5)
N(4)-C(31)	1.383(18)	O(2)-Ru(1)-N(3)	96.6(3)
O(2)-C(36)	1.305(18)	O(1)-Ru(1)-N(3)	174.6(4)
C(1)-C(6)	1.417(15)	N(1)-Ru(1)-N(2)	86.4(5)
C(1)-C(2)	1.408(14)	N(4)-Ru(1)-N(2)	172.2(5)
C(2)-C(3)	1.372(14)	O(2)-Ru(1)-N(2)	93.8(4)
C(3)-C(4)	1.402(14)	O(1)-Ru(1)-N(2)	96.9(4)
C(4)-C(5)	1.382(15)	N(3)-Ru(1)-N(2)	77.7(5)
C(5)-C(6)	1.391(15)		
C(31)-C(32)	1.407(15)		
C(32)-C(33)	1.386(17)		
C(33)-C(34)	1.421(15)		
C(34)-C(35)	1.372(15)		

Table S3 Selected bond angles (°) for **2a**, **2b**, **3** and [**3**]$(ClO_4)_2$

Bond angles	**2a**		**2b**		**3**	[**3**]$(ClO_4)_2$
	X-ray	DFT	X-ray	DFT	X-ray	X-ray
N(1)-Ru(1)-N(4)	167.9(2)	165.6	99.61(9)	102.9	100.57(10)	101.27(9)
N(1)-Ru(1)-O(1)	80.35(18)	78.04	80.61(8)	77.07	80.71(9)	77.81(9)
N(4)-Ru(1)-O(1)	92.63(18)	91.43	86.62(8)	88.03	88.22(9)	87.84(9)
N(1)-Ru(1)-O(2)	89.40(18)	91.48	168.70(8)	167.0	165.33(9)	178.09(9)
N(4)-Ru(1)-O(2)	80.08(17)	78.04	80.49(8)	77.15	80.73(9)	77.06(9)
O(1)-Ru(1)-O(2)	84.67(15)	89.52	88.12(7)	89.93	84.74(8)	102.97(8)
N(1)-Ru(1)-N(3)	98.9(2)	99.75	93.30(9)	97.41	103.12(10)	95.78(10)
N(4)-Ru(1)-N(3)	88.9(2)	91.21	102.04(9)	99.94	98.10(10)	99.29(10)
O(1)-Ru(1)-N(3)	175.0(2)	172.7	170.20(9)	173.1	171.79(9)	171.28(9)
O(2)-Ru(1)-N(3)	100.29(18)	95.54	97.74(8)	94.39	91.08(9)	83.63(9)
N(1)-Ru(1)-N(2)	90.4(2)	92.12	89.75(9)	88.69	88.03(10)	96.64(9)
N(4)-Ru(1)-N(2)	100.2(2)	99.79	170.61(9)	168.1	171.05(10)	162.09(10)
O(1)-Ru(1)-N(2)	96.73(18)	95.52	94.20(8)	95.54	95.67(10)	95.54(9)
O(2)-Ru(1)-N(2)	178.5(2)	174.7	90.18(8)	92.12	91.58(9)	85.04(9)
N(3)-Ru(1)-N(2)	78.3(2)	78.49	78.02(9)	77.25	77.35(10)	79.21(10)

Table S4 NBO-charges involving **2a**^{n}

Atom	**2a**	**2a**$^{+}$	**2a**$^{2+}$	**2a**$^{-}$
Ru1	0.741	0.775	0.802	0.860
N1	-0.478	-0.430	-0.382	-0.573
N2	-0.406	-0.409	-0.418	-0.419
N3	-0.412	-0.417	-0.419	-0.413
N4	-0.464	-0.421	-0.351	-0.552
O1	-0.638	-0.574	-0.528	-0.680
O2	-0.645	-0.580	-0.537	-0.679
C1	0.369	0.418	0.494	0.359
C6	0.138	0.174	0.205	0.104
C31	0.143	0.172	0.222	0.119
C36	0.375	0.420	0.497	0.355

Calculated bond order involving **2a**^{n}

Bond	**2a**	**2a**$^{+}$	**2a**$^{2+}$	**2a**$^{-}$
C1-O1	1.191	1.2778	1.4118	1.1472
C36-O2	1.194	1.2844	1.4054	1.1423
C6-N1	1.246	1.3332	1.4813	1.0716
C31-N4	1.246	1.3400	1.4844	1.1102
C1-C6	1.1849	1.1158	1.0421	1.2466
C1-C2	1.2639	1.2236	1.1818	1.3013
C2-C3	1.4881	1.5277	1.5894	1.4367
C3-C4	1.2770	1.2236	1.1493	1.3518
C4-C5	1.4993	1.5386	1.5980	1.4239
C5-C6	1.2669	1.2335	1.1899	1.3474
C31-C36	1.1867	1.1148	1.0425	1.2629
C31-C32	1.2697	1.2307	1.1860	1.3633
C32-C33	1.4966	1.5418	1.5838	1.4190
C33-C34	1.2795	1.2214	1.1514	1.3533
C34-C35	1.4874	1.5310	1.5961	1.4445
C35-C36	1.2639	1.2216	1.1912	1.2906

Natural electron configuration involving **2a**

Ru(1) [core]5S(0.26)4d(6.93)5p(0.02)5d(0.03)6p(0.01)6d(0.01)
N(1) [core]2S(1.29)2p(4.15)3p(0.02)
O(1) [core]2S(1.69)2p(4.95)3p(0.01)
N(2) [core]2S(1.30)2p(4.09)3p(0.01)
N(3) [core]2S(1.30)2p(4.09)3p(0.01)
N(4) [core]2S(1.29)2p(4.17)3p(0.02)
O(2) [core]2S(1.69)2p(4.94)3p(0.01)

Natural electron configuration involving **2a**$^{+}$

Ru(1) [core]5S(0.26)4d(6.89)5p(0.02)5d(0.03)6p(0.01)6d(0.02)
N(1) [core]2S(1.29)2p(4.12)3p(0.02)
O(1) [core]2S(1.67)2p(4.90)3p(0.01)
N(2) [core]2S(1.29)2p(4.10)3p(0.01)
N(3) [core]2S(1.28)2p(4.12)3p(0.01)
N(4) [core]2S(1.29)2p(4.11)3p(0.02)
O(2) [core]2S(1.67)2p(4.89)3p(0.01)

Natural electron configuration involving **2a**$^{2+}$

Ru(1) [core]5S(0.26)4d(6.84)5p(0.01)5d(0.02)6p(0.02)6d(0.02)
N(1) [core]2S(1.29)2p(4.07)3p(0.02)
O(1) [core]2S(1.66)2p(4.86)3p(0.01)
N(2) [core]2S(1.28)2p(4.12)3p(0.01)
N(3) [core]2S(1.28)2p(4.12)3p(0.01)
N(4) [core]2S(1.29)2p(4.04)3p(0.02)
O(2) [core]2S(1.66)2p(4.86)3p(0.01)

Natural electron configuration involving **2a**$^{-}$

Ru(1) [core]5S(0.26)4d(6.74)5p(0.01)5d(0.02)6p(0.02)6d(0.02)
N(1) [core]2S(1.31)2p(4.24)3p(0.02)
O(1) [core]2S(1.70)2p(4.97)3p(0.01)
N(2) [core]2S(1.31)2p(4.08)3p(0.01)
N(3) [core]2S(1.31)2p(4.09)3p(0.01)
N(4) [core]2S(1.29)2p(4.24)3p(0.02)
O(2) [core]2S(1.70)2p(4.97)3p(0.01)

Table S5 NBO-charges involving **2b**^{n}

Atom	**2b**	**2b**$^{+}$	**2b**$^{2+}$	**2b**$^{-}$
Ru1	0.781	0.789	0.779	0.833
N1	-0.492	-0.437	-0.383	-0.581
N2	-0.399	-0.419	-0.424	-0.397
N3	-0.398	-0.417	-0.421	-0.414
N4	-0.483	-0.436	-0.407	-0.552
O1	-0.620	-0.591	-0.543	-0.671
O2	-0.626	-0.577	-0.520	-0.670
C1	0.363	0.428	0.500	0.357
C6	0.117	0.156	0.198	0.110
C31	0.134	0.171	0.215	0.112
C36	0.367	0.435	0.500	0.363

Calculated bond order involving **2b**^{n}

Bond	**2b**	**2b**$^{+}$	**2b**$^{2+}$	**2b**$^{-}$
C1-O1	1.1799	1.2846	1.4124	1.1590
C36-O2	1.1815	1.3035	1.4330	1.1642
C6-N1	1.1805	1.3178	1.4538	1.1241
C31-N4	1.1619	1.3067	1.4440	1.1156
C1-C6	1.1968	1.1140	1.0413	1.2287
C1-C2	1.2755	1.2304	1.1896	1.2982
C2-C3	1.4568	1.5235	1.5804	1.4264
C3-C4	1.3198	1.2371	1.1643	1.3638
C4-C5	1.4451	1.5167	1.5664	1.4103
C5-C6	1.3135	1.2600	1.2247	1.3522
C31-C36	1.2187	1.1203	1.0386	1.2427
C31-C32	1.2962	1.2532	1.2315	1.3387
C32-C33	1.4779	1.5321	1.5595	1.4320
C33-C34	1.2895	1.2148	1.1499	1.3405
C34-C35	1.4910	1.5543	1.6033	1.4499
C35-C36	1.2532	1.2065	1.1711	1.2796

Natural electron configuration involving **2b**

Ru(1) [core]5S(0.27)4d(6.88)5p(0.02)5d(0.01)6p(0.01)6d(0.03)
N(1) [core]2S(1.27)2p(4.20)3p(0.01)
O(1) [core]2S(1.67)2p(4.94)3p(0.01)
N(2) [core]2S(1.29)2p(4.09)3p(0.02)
N(3) [core]2S(1.29)2p(4.08)3p(0.02)
N(4) [core]2S(1.28)2p(4.18)3p(0.02)
O(2) [core]2S(1.68)2p(4.94)3p(0.01)

Natural electron configuration involving **2b**$^{+}$

Ru(1) [core]5S(0.26)4d(6.89)5p(0.02)5d(0.03)6p(0.01)6d(0.01)
N(1) [core]2S(1.29)2p(4.13)3p(0.01)
O(1) [core]2S(1.68)2p(4.90)3p(0.01)
N(2) [core]2S(1.30)2p(4.10)3p(0.01)
N(3) [core]2S(1.30)2p(4.09)3p(0.02)
N(4) [core]2S(1.30)2p(4.12)3p(0.02)
O(2) [core]2S(1.68)2p(4.89)3p(0.01)

Natural electron configuration involving **2b**$^{2+}$

Ru(1) [core]5S(0.26)4d(6.91)5d(0.01)6p(0.02)6d(0.02)
N(1) [core]2S(1.30)2p(4.06)3p(0.02)
O(1) [core]2S(1.67)2p(4.86)3p(0.01)
N(2) [core]2S(1.29)2p(4.11)3p(0.01)
N(3) [core]2S(1.30)2p(4.10)3p(0.02)
N(4) [core]2S(1.30)2p(4.08)3p(0.02)
O(2) [core]2S(1.68)2p(4.84)3p(0.01)

Natural electron configuration involving **2b**$^{-}$

Ru(1) [core]5S(0.26)4d(6.77)5p(0.02)5d(0.03)6p(0.01)6d(0.01)
N(1) [core]2S(1.30)2p(4.26)3p(0.02)
O(1) [core]2S(1.68)2p(4.98)3p(0.01)
N(2) [core]2S(1.31)2p(4.07)3p(0.01)
N(3) [core]2S(1.32)2p(4.08)3p(0.02)
N(4) [core]2S(1.29)2p(4.24)3p(0.02)
O(2) [core]2S(1.68)2p(4.98)3p(0.01)

Table S6a Selected molecular orbitals along with their energies and compositions for **2a** in triplet (S=1) state

		α-spin		
MO	Energy, eV	Composition		
		Q'_2	Ru	bpy
LUMO+3	-0.95	86	12	02
LUMO+2	-1.41	02	03	95
LUMO+1	-1.57	05	04	91
LUMO	-2.41	01	07	92
SOMO1	-4.27	75	24	01
SOMO2	-4.90	96	03	01
HOMO-2	-5.15	40	56	04
HOMO-3	-5.59	41	48	11
		β- spin		
LUMO+3	-1.56	05	05	90
LUMO+2	-2.35	65	27	08
LUMO+1	-2.40	04	11	85
LUMO	-3.25	94	04	02
HOMO	-4.82	48	49	03
HOMO-1	-5.18	39	46	15
HOMO-2	-5.32	49	47	04
HOMO-3	-5.71	75	19	06

Table S6b Selected molecular orbitals along with their energies and compositions for **2a** in BS(1,1) state

		α-spin			
MO	Energy, eV	Composition			
		$(Q'_2)1$	$(Q'_2)2$	Ru	bpy
LUMO+3	-1.58	02	01	03	94
LUMO+2	-1.76	01	02	04	93
LUMO+1	-2.56	01	01	09	89
LUMO	-2.86	06	66	24	04
SOMO	-4.60	67	22	10	01
HOMO-1	-4.98	13	44	49	04
HOMO-2	-5.45	19	15	53	13
HOMO-3	-5.85	30	38	28	04
		β- spin			
LUMO+3	-1.58	01	01	03	95
LUMO+2	-1.76	01	02	04	93
LUMO+1	-2.56	02	01	09	88
LUMO	-2.86	66	07	22	05
SOMO	-4.59	22	67	10	01
HOMO-1	-4.98	33	14	50	03
HOMO-2	-5.45	16	19	52	13
HOMO-3	-5.87	36	31	29	04

Table S7 Selected molecular orbitals along with their energies and compositions for **2b** in triplet (S=1) state

α-Spin				
MO	Energy, eV	Composition		
		Q'_2	Ru	bpy
LUMO+5	-0.65	93	05	02
LUMO+4	-0.73	95	04	01
LUMO+3	-0.77	89	09	02
LUMO+2	-1.32	02	02	96
LUMO+1	-1.51	02	04	94
LUMO	-2.38	01	06	93
SOMO1	-4.18	74	25	01
SOMO2	-4.83	93	05	02
HOMO-2	-5.15	43	55	02
HOMO-3	-5.41	42	49	09
HOMO-4	-5.84	64	32	04
HOMO-5	-6.13	72	26	02
β-Spin				
LUMO+5	-0.70	95	04	01
LUMO+4	-1.29	05	05	90
LUMO+3	-1.50	02	04	94
LUMO+2	-2.22	61	30	09
LUMO+1	-2.37	03	08	89
LUMO	-3.23	96	03	01
HOMO	-4.78	47	50	03
HOMO-1	-5.04	56	36	08
HOMO-2	-5.23	43	51	06
HOMO-3	-5.70	70	26	04
HOMO-4	-5.94	64	35	01
HOMO-5	-6.65	96	03	01

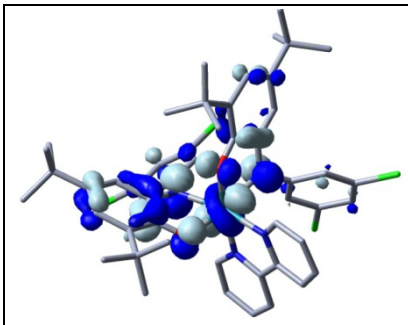
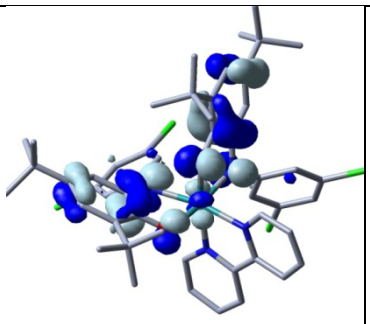
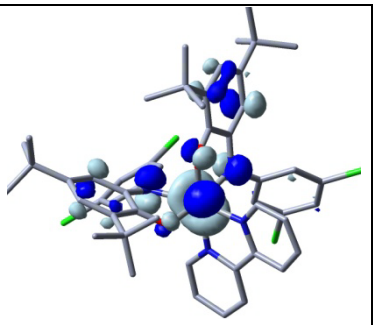
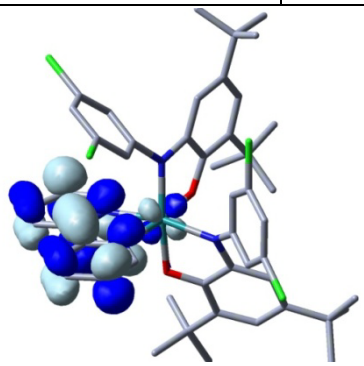
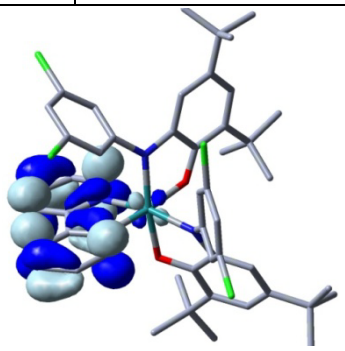
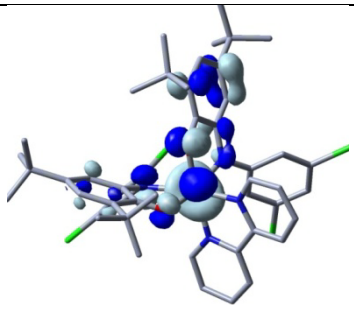
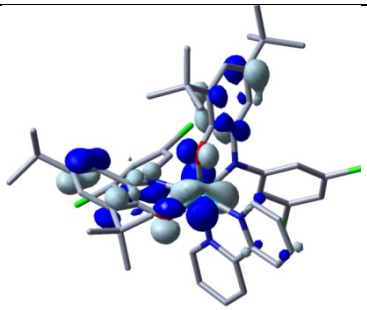
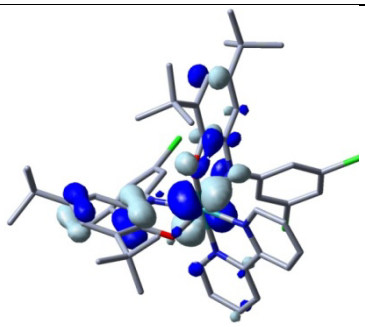
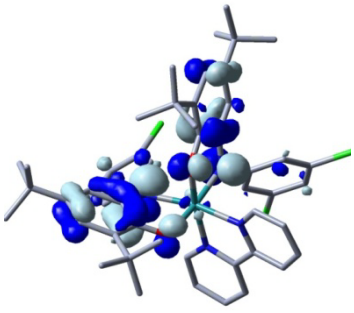
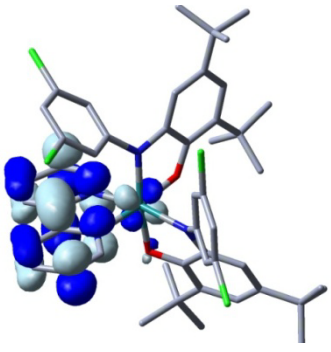
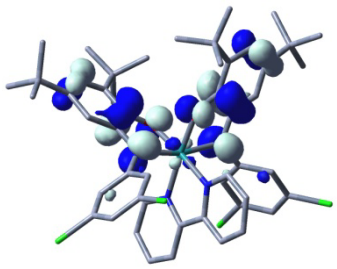
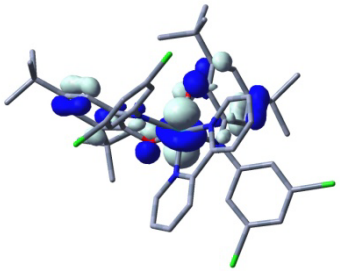
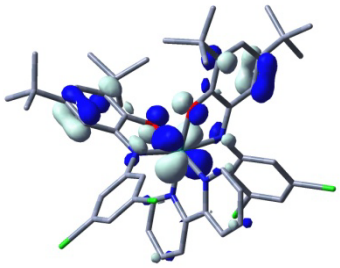
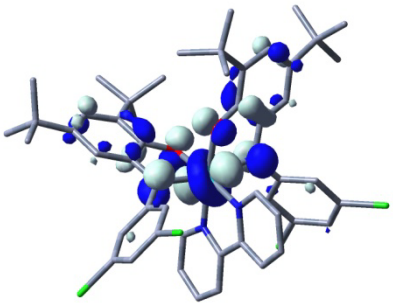
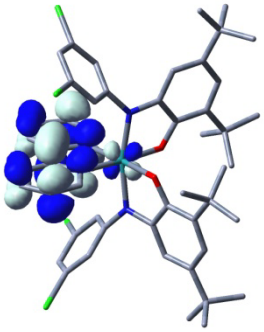
		
SOMO1	SOMO2	HOMO-2
		
LUMO	LUMO+1	
α-MO of **2b**		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	
β-MO of **2b**		

Table S8 Selected molecular orbitals along with their energies and compositions for **2a**$^{+}$ (S=1/2 state)

α-spin				
MO	Energy, eV	Composition		
		Q'_2	Ru	bpy
LUMO+5	-3.29	95	04	01
LUMO+4	-3.54	79	19	02
LUMO+3	-3.98	01	03	96
LUMO+2	-4.14	03	03	94
LUMO+1	-5.04	01	05	94
LUMO	-5.85	61	37	02
SOMO	-7.49	96	04	0
HOMO-1	-8.10	50	47	03
HOMO-2	-8.42	46	45	09
HOMO-3	-8.68	55	41	04
HOMO-4	-8.82	71	24	05
HOMO-5	-9.06	62	35	03
HOMO-6	-9.35	99	01	01
HOMO-7	-9.36	97	02	01
HOMO-8	-9.46	98	02	0
HOMO-9	-9.60	97	02	01
HOMO-10	-9.85	02	01	97
β- spin				
LUMO+5	-3.53	78	20	02
LUMO+4	-3.99	01	02	97
LUMO+3	-4.14	03	03	94
LUMO+2	-5.04	01	05	94
LUMO+1	-5.55	85	14	01
LUMO	-6.05	96	02	01
HOMO	-8.05	61	37	02
HOMO-1	-8.34	66	28	05
HOMO-2	-8.76	52	40	08
HOMO-3	-8.84	43	53	04
HOMO-4	-9.03	52	44	04
HOMO-5	-9.32	98	01	01
HOMO-6	-9.34	97	01	02
HOMO-7	-9.41	98	02	0
HOMO-8	-9.57	95	04	01
HOMO-9	-9.85	02	01	97
HOMO-10	-10.21	97	02	01

		
SOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	
α -MO of **2a**$^{+}$		

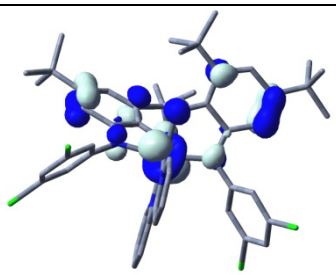
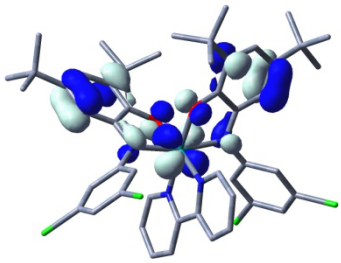
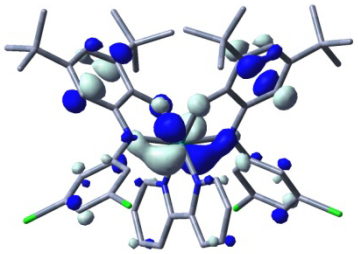
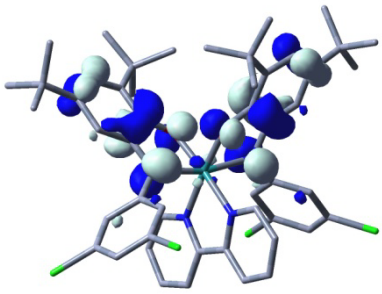
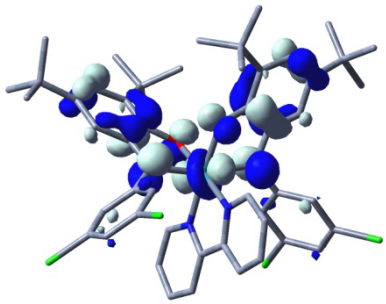
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	
β-MO of **2a**$^{+}$		

Table S9 Selected molecular orbitals along with their energies and compositions for **2b**$^{+}$ (S=1/2 state)

α-spin				
MO	Energy, eV	Composition		
		Q'_2	Ru	bpy
LUMO+5	-3.43	92	07	01
LUMO+4	-3.62	74	22	04
LUMO+3	-3.92	01	04	95
LUMO+2	-4.09	01	03	96
LUMO+1	-5.04	01	06	93
LUMO	-5.95	60	39	01
SOMO	-7.51	97	03	0
HOMO-1	-8.26	47	51	02
HOMO-2	-8.36	50	47	03
HOMO-3	-8.68	55	42	03
HOMO-4	-8.97	63	31	06
HOMO-5	-9.13	63	34	03
β- spin				
LUMO+5	-3.60	75	22	03
LUMO+4	-3.93	02	02	96
LUMO+3	-4.09	02	03	95
LUMO+2	-5.04	01	04	95
LUMO+1	-5.55	83	16	01
LUMO	-6.18	98	02	0
HOMO	-8.15	57	41	02
HOMO-1	-8.20	67	29	04
HOMO-2	-8.61	41	50	09
HOMO-3	-8.88	51	43	06
HOMO-4	-9.08	55	41	04
HOMO-5	-9.30	95	03	02

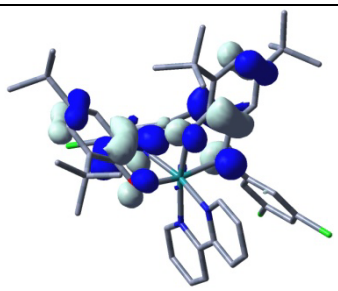
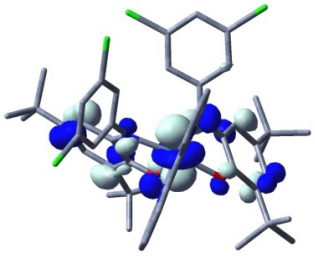
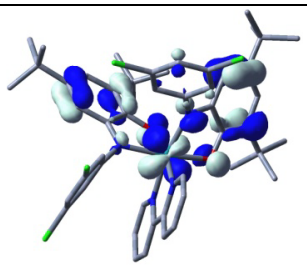
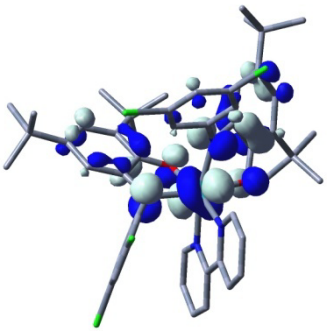
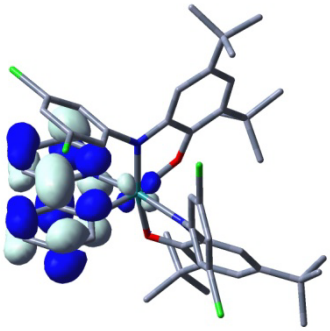
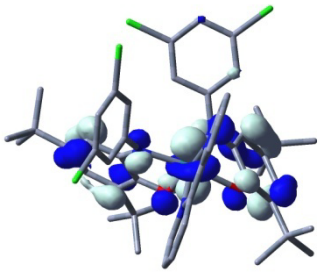
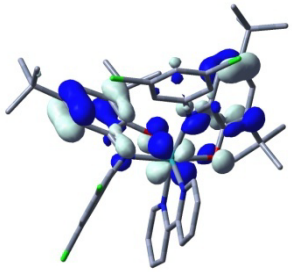
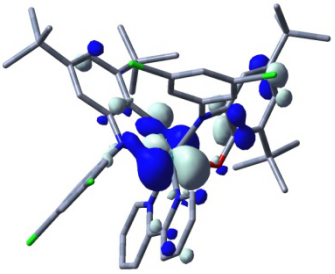
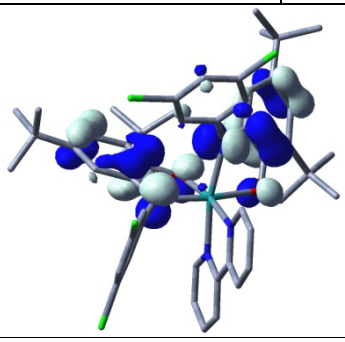
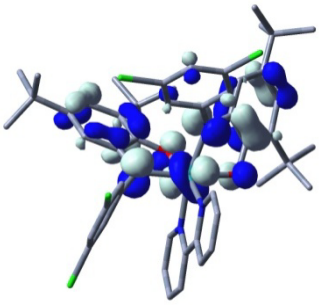
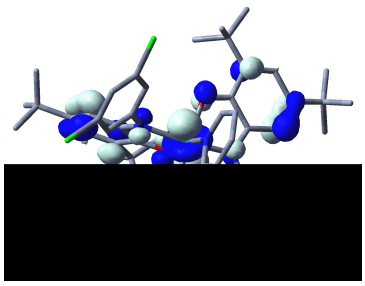
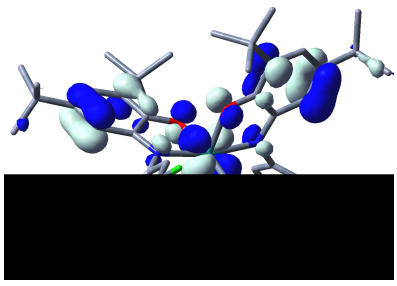
		
SOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	
α-MO of **2b**$^{+}$		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	
β-MO of **2b**$^{+}$		

Table S10 Some selected molecular orbitals along with their energies and compositions for **2a**$^{2+}$ (S=0 state)

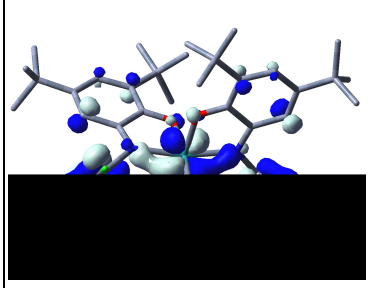
MO	Energy, eV	Composition		
		Q'_2	Ru	bpy
LUMO+5	-6.31	64	30	06
LUMO+4	-6.67	03	01	96
LUMO+3	-6.84	03	02	95
LUMO+2	-7.74	01	04	95
LUMO+1	-9.00	82	17	01
LUMO	-9.29	90	08	02
HOMO	-11.27	61	37	02
HOMO-1	-11.46	68	28	04
HOMO-2	-11.81	74	22	04
HOMO-3	-11.88	91	08	01
HOMO-4	-11.91	98	02	0
HOMO-5	-11.96	49	46	05
HOMO-6	-12.18	79	19	02
HOMO-7	-12.22	85	12	03
HOMO-8	-12.23	66	31	03
HOMO-9	-12.67	02	01	97
HOMO-10	-12.96	99	01	0



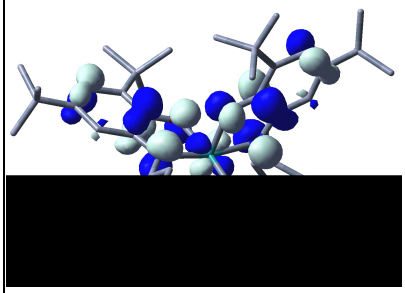
HOMO



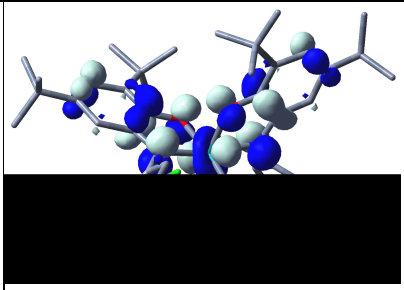
HOMO-1



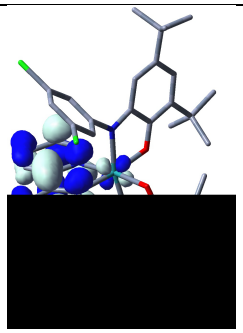
HOMO-2



LUMO



LUMO+1

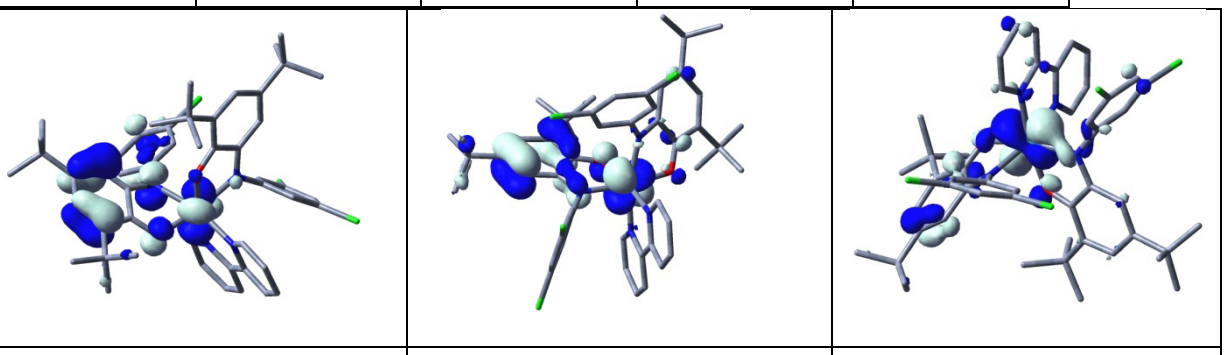


LUMO+2

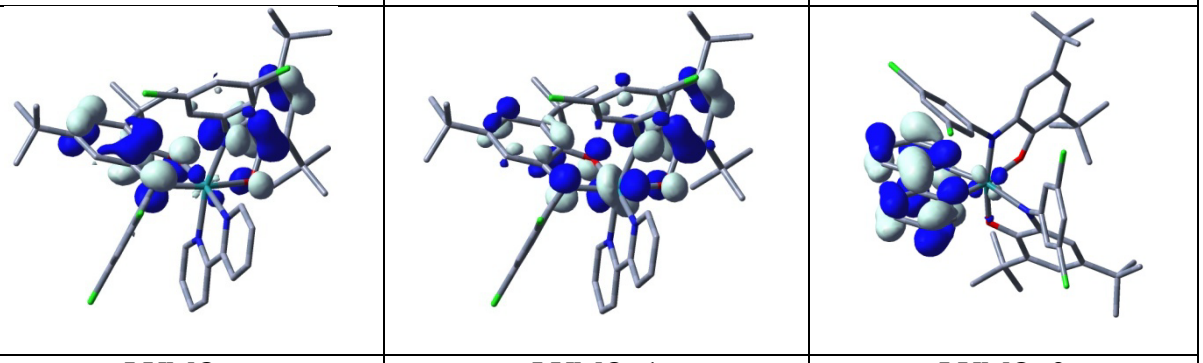
MO of **2a**$^{2+}$

Table S11 Some selected molecular orbitals along with their energies and compositions for **2b**$^{2+}$ (S=0 state)

MO	Energy, eV	Composition		
		Q'_2	Ru	bpy
LUMO+5	-6.31	12	23	65
LUMO+4	-6.41	08	24	68
LUMO+3	-6.48	16	36	48
LUMO+2	-7.42	01	05	94
LUMO+1	-8.69	78	21	01
LUMO	-9.29	91	07	02
HOMO	-11.13	53	46	01
HOMO-1	-11.20	57	39	04
HOMO-2	-11.52	75	20	05
HOMO-3	-11.63	93	06	01
HOMO-4	-11.72	95	04	01
HOMO-5	-11.84	44	52	04



HOMO | HOMO-1 | HOMO-2



LUMO | LUMO+1 | LUMO+2

MO of **2b**$^{2+}$

Table S12 Some selected molecular orbitals along with their energies and compositions for **2a**$^{-}$ (S=1/2 state)

α-spin				
MO	Energy, eV	Composition		
		Q'_2	Ru	bpy
LUMO+5	1.67	92	08	0
LUMO+4	1.59	97	02	01
LUMO+3	1.52	95	04	01
LUMO+2	1.04	02	03	95
LUMO+1	0.93	04	05	91
LUMO	0.01	03	11	86
SOMO	-1.45	83	16	01
HOMO-1	-1.74	89	07	04
HOMO-2	-2.40	49	48	03
HOMO-3	-2.79	60	30	10
HOMO-4	-3.23	61	29	10
HOMO-5	-3.33	57	37	06
HOMO-6	-3.51	56	41	03
HOMO-7	-4.04	99	01	0
HOMO-8	-4.31	94	03	03
HOMO-9	-4.56	98	01	01
HOMO-10	-4.61	97	01	02
β- spin				
LUMO+5	1.59	98	01	01
LUMO+4	1.53	97	02	01
LUMO+3	1.07	03	05	92
LUMO+2	0.94	04	05	91
LUMO+1	0.07	16	23	61
LUMO	0.04	25	26	49
HOMO	-1.46	90	06	04
HOMO-1	-2.17	49	48	03
HOMO-2	-2.60	57	32	11
HOMO-3	-2.64	59	38	03
HOMO-4	-3.11	63	28	09
HOMO-5	-3.32	66	31	03
HOMO-6	-3.98	99	01	0
HOMO-7	-4.23	95	03	02
HOMO-8	-4.53	97	01	02
HOMO-9	-4.56	94	04	02
HOMO-10	-4.58	83	08	09

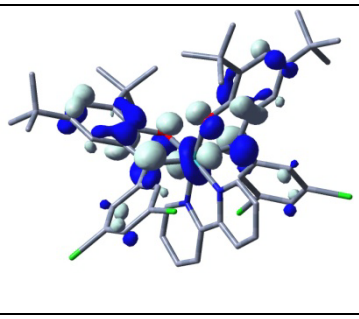
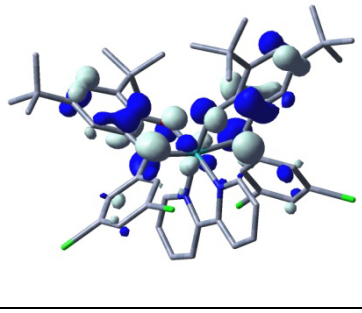
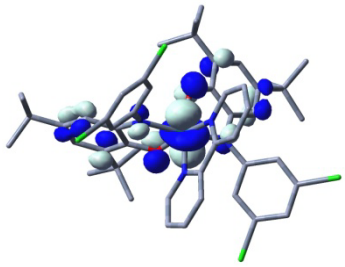
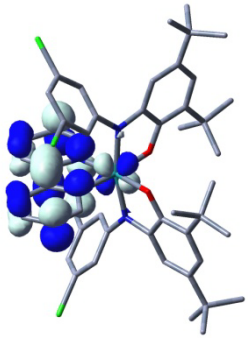
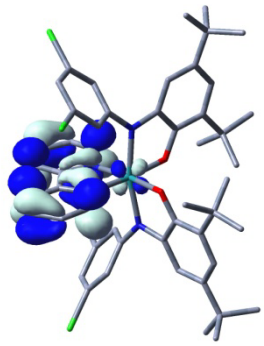
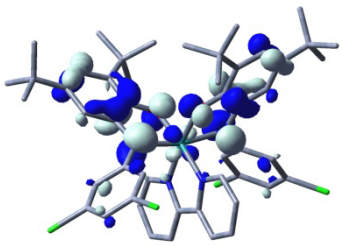
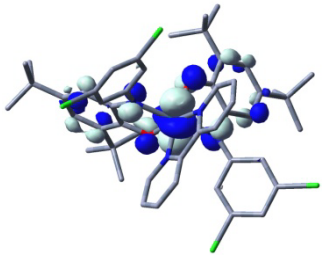
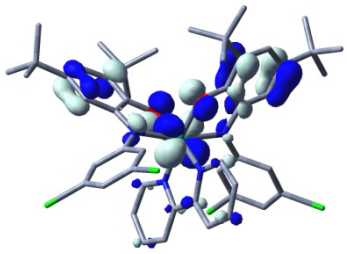
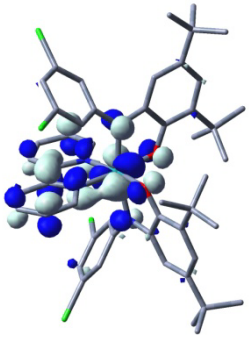
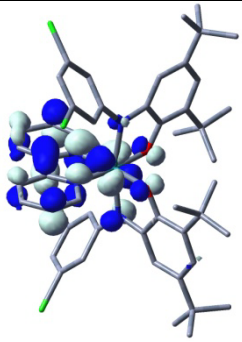
		
SOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	
α-MO of **2a**$^{-}$		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	
β-MO of **2a**$^{-}$		

Table S13 Some selected molecular orbitals along with their energies and compositions for **2b**$^{-}$ (S=1/2 state)

α-spin				
MO	Energy, eV	Composition		
		Q'_2	Ru	bpy
LUMO+5	1.97	87	10	03
LUMO+4	1.86	97	02	01
LUMO+3	1.79	93	05	02
LUMO+2	0.92	01	02	97
LUMO+1	0.77	01	03	96
LUMO	-0.15	02	12	86
SOMO	-1.39	82	17	01
HOMO-1	-1.79	95	04	01
HOMO-2	-2.45	47	50	03
HOMO-3	-2.66	59	32	09
HOMO-4	-3.10	60	30	10
HOMO-5	-3.30	58	36	06
β- spin				
LUMO+5	1.89	96	03	01
LUMO+4	1.88	95	04	01
LUMO+3	0.96	03	06	91
LUMO+2	0.78	02	06	92
LUMO+1	0.03	48	44	18
LUMO	-0.13	08	18	74
HOMO	-1.45	92	05	03
HOMO-1	-2.24	46	52	02
HOMO-2	-2.44	56	35	09
HOMO-3	-2.66	57	40	03
HOMO-4	-3.00	67	26	07
HOMO-5	-3.22	64	33	03

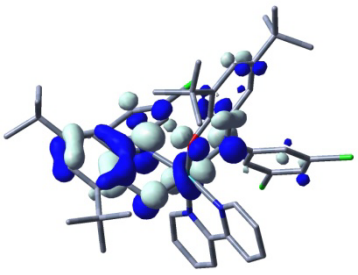
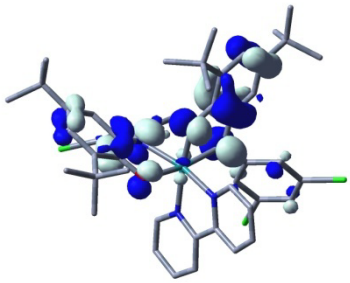
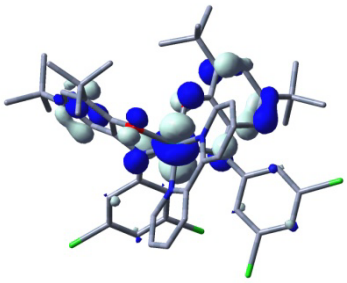
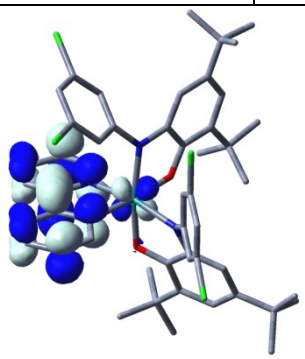
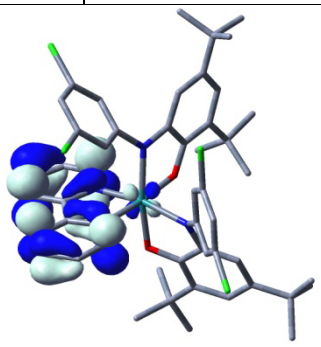
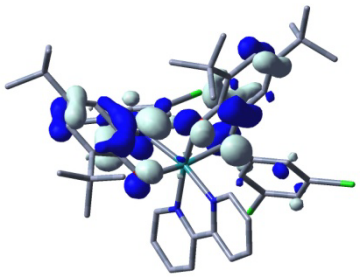
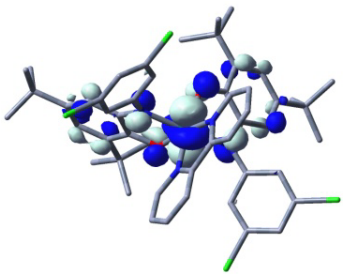
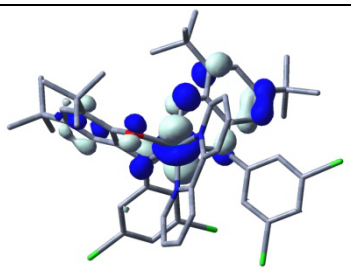
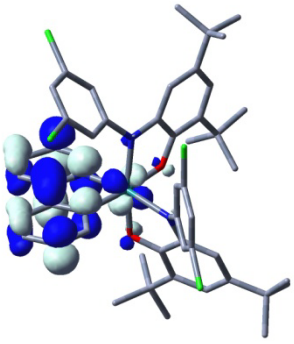
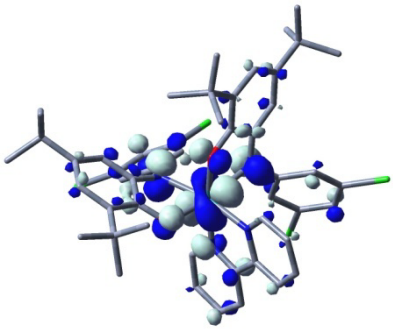
		
SOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	
α-MO of **2b**$^{-}$		
		
HOMO	HOMO-1	HOMO-2
		
LUMO	LUMO+1	
β-MO of **2b**$^{-}$		

Table S14 DFT calculated selected bond distances (Å) and angles (°) in **2a**, $\mathbf{2a}^{+}$, $\mathbf{2a}^{2+}$ and $\mathbf{2a}^{-}$

Bond distances	**2a**	$\mathbf{2a}^{+}$	$\mathbf{2a}^{2+}$	$\mathbf{2a}^{-}$
Ru(1)-N(1)	2.046	2.062	2.071	2.102
Ru(1)-N(2)	2.059	2.077	2.082	2.089
Ru(1)-N(3)	2.059	2.078	2.082	2.075
Ru(1)-N(4)	2.045	2.061	2.071	2.095
Ru(1)-O(1)	2.049	2.049	2.072	2.105
Ru(1)-O(2)	2.050	2.050	2.071	2.102
C(1)-O(1)	1.323	1.298	1.274	1.369
C(36)-O(2)	1.324	1.298	1.274	1.369
C(6)-N(1)	1.378	1.352	1.327	1.431
C(31)-N(4)	1.379	1.352	1.328	1.419
C(1)-C(6)	1.437	1.454	1.478	1.431
C(1)-C(2)	1.426	1.416	1.427	1.434
C(2)-C(3)	1.389	1.377	1.367	1.407
C(3)-C(4)	1.422	1.425	1.445	1.423
C(4)-C(5)	1.382	1.373	1.362	1.406
C(5)-C(6)	1.415	1.428	1.441	1.408
C(31)-C(32)	1.415	1.428	1.441	1.412
C(32)-C(33)	1.382	1.373	1.362	1.406
C(33)-C(34)	1.422	1.425	1.445	1.422
C(34)-C(35)	1.390	1.378	1.368	1.408
C(35)-C(36)	1.426	1.416	1.427	1.430
C(31)-C(36)	1.437	1.453	1.477	1.432
Bond angles				
N(1)-Ru(1)-N(2)	92.12	90.77	90.69	88.73
N(1)-Ru(1)-N(3)	99.75	100.1	98.72	101.2
N(1)-Ru(1)-N(4)	165.6	166.2	167.8	166.4
N(1)-Ru(1)-O(1)	78.04	78.85	77.46	78.35
N(1)-Ru(1)-O(2)	91.48	91.30	93.93	93.16
N(2)-Ru(1)-N(3)	78.49	78.04	78.38	78.25
N(2)-Ru(1)-N(4)	99.79	99.89	98.72	100.3
N(2)-Ru(1)-O(1)	95.52	96.83	95.53	98.43
N(2)-Ru(1)-O(2)	174.7	175.1	172.9	173.8
N(3)-Ru(1)-N(4)	91.21	90.65	90.69	90.62
N(3)-Ru(1)-O(1)	172.7	174.8	172.8	176.6
N(3)-Ru(1)-O(2)	95.54	96.80	95.56	95.67
N(4)-Ru(1)-O(1)	91.43	91.16	93.93	90.23
N(4)-Ru(1)-O(2)	78.04	78.83	77.47	78.86
O(1)-Ru(1)-O(2)	89.52	88.34	90.74	87.64

Table S15 DFT calculated selected bond distances (Å) and angles (°) in **2b**, $\mathbf{2b}^{+}$, $\mathbf{2b}^{2+}$ and $\mathbf{2b}^{-}$

Bond distances	**2b**	$\mathbf{2b}^{+}$	$\mathbf{2b}^{2+}$	$\mathbf{2b}^{-}$
Ru(1)-N(1)	2.039	2.064	2.072	2.105
Ru(1)-N(2)	2.081	2.107	2.117	2.089
Ru(1)-N(3)	2.080	2.107	2.112	2.118
Ru(1)-N(4)	2.043	2.106	2.123	2.096
Ru(1)-O(1)	2.040	2.105	2.119	2.089
Ru(1)-O(2)	2.048	2.098	2.109	2.109
C(1)-O(1)	1.325	1.301	1.278	1.345
C(36)-O(2)	1.322	1.299	1.275	1.343
C(6)-N(1)	1.389	1.354	1.334	1.417
C(31)-N(4)	1.387	1.351	1.337	1.416
C(1)-C(6)	1.434	1.460	1.483	1.433
C(1)-C(2)	1.411	1.428	1.433	1.431
C(2)-C(3)	1.386	1.382	1.374	1.404
C(3)-C(4)	1.419	1.439	1.447	1.412
C(4)-C(5)	1.390	1.376	1.371	1.400
C(5)-C(6)	1.432	1.420	1.424	1.409
C(31)-C(32)	1.412	1.422	1.423	1.412
C(32)-C(33)	1.382	1.374	1.368	1.397
C(33)-C(34)	1.423	1.431	1.444	1.417
C(34)-C(35)	1.385	1.376	1.369	1.399
C(35)-C(36)	1.436	1.434	1.443	1.434
C(31)-C(36)	1.441	1.461	1.491	1.433
Bond angles				
N(1)-Ru(1)-N(2)	88.69	90.86	91.09	88.73
N(1)-Ru(1)-N(3)	97.41	95.34	96.74	101.2
N(1)-Ru(1)-N(4)	102.9	101.0	103.7	166.4
N(1)-Ru(1)-O(1)	77.07	77.83	76.55	78.35
N(1)-Ru(1)-O(2)	167.0	166.3	164.0	93.16
N(2)-Ru(1)-N(3)	77.25	77.20	77.45	78.25
N(2)-Ru(1)-N(4)	168.1	168.0	165.1	100.3
N(2)-Ru(1)-O(1)	95.54	95.60	98.83	98.43
N(2)-Ru(1)-O(2)	92.12	91.04	89.99	173.8
N(3)-Ru(1)-N(4)	99.94	101.4	100.2	90.62
N(3)-Ru(1)-O(1)	173.1	170.1	172.1	176.6
N(3)-Ru(1)-O(2)	94.39	98.27	99.04	95.67
N(4)-Ru(1)-O(1)	88.03	86.96	85.55	90.23
N(4)-Ru(1)-O(2)	77.15	77.35	75.78	78.86
O(1)-Ru(1)-O(2)	89.93	88.52	87.54	87.64

Table S16 TD-DFT of **2a**, **2a**$^{+}$, **2a**$^{2+}$ and **2a**$^{-}$

For **2a**:

Excitation Energy(eV)	Wavelength (nm)	f	Transition	Character
1.0981	1129.1	0.0011	(87%)HOMO(β) → LUMO(β)	Ru(dπ)/(Q'_2)(π) → (Q'_2)(π*)
1.1603	1068.6	0.0045	(96%)SOMO1 → LUMO(α)	(Q'_2)(π) → bpy(π*)
1.2977	955.4	0.0214	(63%)SOMO2 → LUMO(α)	(Q'_2)(π) → bpy(π*)
1.6477	752.5	0.0753	(43%)HOMO-2(β) → LUMO(β) (46%)HOMO-1(β) → LUMO+1(β)	Ru(dπ)/(Q'_2)(π) → (Q'_2)(π*) Ru(dπ)/(Q'_2)(π) → bpy(π*)
1.8010	688.4	0.0428	(48%)HOMO-1(β) → LUMO+2(β) (22%)HOMO-2(β) → LUMO+1(β)	Ru(dπ)/(Q'_2)(π) → bpy(π*)
2.1894	566.3	0.0513	(53%)HOMO-3(α) → LUMO+1(α) (27%)HOMO-2(β) → LUMO+3(β)	Ru(dπ)/(Q'_2)(π) → bpy(π*)

For **2a**$^{+}$:

Excitation Energy(eV)	Wavelength (nm)	f	Transition	Character
1.0032	1235.9	0.0189	(76%)HOMO(β) → LUMO(β)	Ru(dπ)/(Q'_2)(π) → (Q'_2)(π*)
1.2145	1020.8	0.0328	(40%)HOMO-2(α) → LUMO(α) (25%)SOMO → LUMO(α)	Ru(dπ)/(Q'_2)(π) → (Q'_2)(π*)/Ru(dπ) (Q'_2)(π) → (Q'_2)(π*)/Ru(dπ)
1.3267	934.6	0.0098	(60%)HOMO-1(β) → LUMO(β)	Ru(dπ)/(Q'_2)(π) → (Q'_2)(π*)
1.8457	671.7	0.2001	(43%)HOMO-3(β) → LUMO(β)	Ru(dπ)/(Q'_2)(π) → (Q'_2)(π*)
2.4505	505.9		(48%)HOMO-2(β) → LUMO+1(β) (22%)HOMO-3(β) → LUMO+1(β)	Ru(dπ)/(Q'_2)(π) → (Q'_2)(π*)

For **2a**$^{2+}$:

Excitation Energy(eV)	Wavelength (nm)	f	Transition	Character
1.2301	1007.9	0.0031	(84%)HOMO → LUMO	Ru(dπ)/(Q$'_2$)(π) → (Q$'_2$)(π^*)
1.5915	779.0	0.0040	(73%)HOMO-1 → LUMO	Ru(dπ)/(Q$'_2$)(π) → (Q$'_2$)(π^*)
1.9204	645.6	0.2040	(84%)HOMO-2 → LUMO	Ru(dπ)/(Q$'_2$)(π) → (Q$'_2$)(π^*)
2.0673	599.7	0.0981	(42%)HOMO-3 → LUMO (21%)HOMO-1 → LUMO+1	(Q$'_2$)(π) → (Q$'_2$)(π^*) Ru(dπ)/(Q$'_2$)(π) → (Q$'_2$)^2(π^*)
2.4179	512.8	0.1659	(48%)HOMO-6 → LUMO (22%)HOMO-2 → LUMO+1	Ru(dπ)/(Q$'_2$)(π) → (Q$'_2$)(π^*)

For **2a**$^{-}$:

Excitation Energy(eV)	Wavelength (nm)	f	Transition	Character
0.6887	1800.3	0.0282	(49%)SOMO → LUMO(α) (43%)HOMO(β) → LUMO+1(β)	(Q$'_2$)(π) → bpy(π^*)
0.8003	1549.2	0.0383	(49%)SOMO→ LUMO(α) (36%)HOMO(β) → LUMO+1(β)	(Q$'_2$)(π) → bpy(π^*)
1.2814	967.5	0.0175	(88%)HOMO-1(β) → LUMO(β)	Ru(dπ)/(Q$'_2$)(π) → bpy(π^*)
1.4655	846.0	0.0544	(72%)HOMO-2(β) → LUMO+1(β)	Ru(dπ)/(Q$'_2$)(π) → bpy(π^*)
1.7295	716.9	0.0416	(81%)HOMO-3(β) → LUMO+1(β)	Ru(dπ)/(Q$'_2$)(π) → bpy(π^*)
1.7937	691.2	0.0125	(87%)HOMO-3(β) → LUMO(β)	Ru(dπ)/(Q$'_2$)(π) → bpy(π^*)
1.9766	627.2	0.0513	(87%)HOMO-4(β) → LUMO+1(β)	Ru(dπ)/(Q$'_2$)(π) → bpy(π^*)

Table S17 TD-DFT of **2b**, **2b**$^{+}$, **2b**$^{2+}$ and **2b**$^{-}$

For **2b**:

Excitation Energy(eV)	Wavelength (nm)	f	Transition	Character
1.0342	1198.8	0.0054	(96%)SOMO1 → LUMO(α)	Ru(dπ)/(Q′$_2$)(π) → bpy(π*)
1.2294	1008.5	0.0091	(96%)HOMO(β) → LUMO(β)	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)
1.3213	938.4	0.0915	(63%)HOMO-1(β) → LUMO(β)	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)
1.5907	779.4	0.0168	(60%)HOMO-1(β) → LUMO+1(β) (22%)HOMO-2(β) → LUMO+1(β)	Ru(dπ)/(Q′$_2$)(π) → bpy(π*)
1.8764	660.8	0.0180	(88%)HOMO-4(β) → LUMO(β)	Ru(dπ)/(Q′$_2$)(π) → bpy(π*)
2.1759	569.8	0.0455	(41%)HOMO-2(β) → LUMO+1(β) (37%)HOMO-4(β) → LUMO+1(β)	Ru(dπ)/(Q′$_2$)(π) → bpy(π*)

For **2b**$^{+}$:

Excitation Energy(eV)	Wavelength (nm)	f	Transition	Character
1.0463	1184.9	0.0163	(45%)SOMO → LUMO(α) (42%)HOMO(β) → LUMO(β)	(Q′$_2$)(π) → (Q′$_2$)(π*)/Ru(dπ) Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)
1.2782	970.0	0.0289	(46%)HOMO-1(β) → LUMO(β) (21%)HOMO-1(α) → LUMO(α)	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*) Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)/Ru(dπ)
1.7633	703.1	0.0211	(49%)HOMO-1(β) → LUMO+1(β) (22%)HOMO-2(β) → LUMO+1(β)	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)
1.8170	682.3	0.1206	(63%)HOMO-2(β) → LUMO+1(β)	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)
2.0619	601.3	0.0452	(41%)HOMO-3(β) → LUMO+1(β) (37%)HOMO-2(α) → LUMO(α)	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*) Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)/Ru(dπ)
2.4150	513.4	0.0339	(79%)HOMO-4(β) → LUMO+1(β)	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)

For **2b**$^{2+}$:

Excitation Energy(eV)	Wavelength (nm)	f	Transition	Character
1.3066	948.9	0.0318	(57%)HOMO → LUMO (23%)HOMO-1 → LUMO	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)
1.6721	741.5	0.0368	(79%)HOMO-2 → LUMO	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)
1.7528	707.3	0.0355	(82%)HOMO-3 → LUMO	(Q′$_2$)(π) → (Q′$_2$)(π*)
1.8778	660.2	0.1589	(44%)HOMO-4 → LUMO (32%)HOMO-5 → LUMO	(Q′$_2$)(π) → (Q′$_2$)(π*) Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)
2.4155	513.3	0.108	(42%)HOMO-2 → LUMO+1 (23%)HOMO-7 → LUMO	Ru(dπ)/(Q′$_2$)(π) → (Q′$_2$)(π*)

For **2b**$^{-}$:

Excitation Energy(eV)	Wavelength (nm)	f	Transition	Character
0.7840	1581.4	0.0355	(43%)HOMO(β) → LUMO(β) (34%)HOMO-1(β) → LUMO(β)	(Q′$_2$)(π) → bpy(π*) Ru(dπ)/(Q′$_2$)(π) → bpy(π*)
0.9182	1350.3	0.0365	(50%)HOMO-1(β) → LUMO(β) (20%)HOMO(β) → LUMO(β)	Ru(dπ)/(Q′$_2$)(π) → bpy(π*) (Q′$_2$)(π) → bpy(π*)
0.9603	1291.1	0.0143	(81%)SOMO → LUMO(α)	(Q′$_2$)(π) → bpy(π*)
1.2415	998.7	0.0544	(63%)HOMO-2(β) → LUMO(β)	Ru(dπ)/(Q′$_2$)(π) → bpy(π*)
1.7191	721.2	0.0812	(67%)HOMO-3(β) → LUMO(β)	Ru(dπ)/(Q′$_2$)(π) → bpy(π*)
2.0029	619.0	0.0319	(61%)HOMO-2(α) → LUMO(α)	Ru(dπ)/(Q′$_2$)(π) → bpy(π*)
2.1602	573.9	0.0482	(64%)HOMO-4(β) → LUMO(β)	Ru(dπ)/(Q′$_2$)(π) → bpy(π*)

Table S18 Optimised cartesian coordinates of **2a** (DFT/UB3LYP/SDD/6-31G(d))

(Triplet state, S=1)

E(Total)= −2461.81377411 a.u.

Ru	-0.000500	-0.419300	-0.010700
Cl	5.754300	-3.598600	-1.186500
Cl	3.213400	-0.823500	-5.133200
Cl	-5.771800	-3.646400	0.916500
Cl	-3.226300	-1.183100	5.062400
O	0.342800	0.917300	1.505400
O	-0.335000	1.024500	-1.426100
N	2.022000	-0.153700	-0.154800
N	0.222900	-2.060600	1.213700
N	-0.234500	-1.966200	-1.350300
N	-2.022800	-0.151500	0.149200
C	1.592000	1.341100	1.618300
C	2.007900	2.331900	2.557900
C	3.355200	2.673400	2.557600
H	3.689900	3.424900	3.261500
C	4.325800	2.113500	1.682500
C	3.912700	1.159500	0.771400
H	4.610800	0.718500	0.071700
C	2.558200	0.758300	0.729800
C	5.782900	2.595700	1.772300
C	6.696000	1.891000	0.751100
H	6.721100	0.806800	0.909300
H	7.720800	2.265500	0.854000
H	6.374800	2.080900	-0.279300
C	6.337800	2.309300	3.189200
H	5.750200	2.810100	3.965700
H	7.372700	2.663900	3.270600
H	6.327000	1.233800	3.400600
C	5.843100	4.118900	1.498300
H	5.462600	4.348300	0.496500
H	6.878600	4.475300	1.561700
H	5.248600	4.687000	2.221100
C	1.002400	3.005000	3.509900
C	1.673700	4.065200	4.404600
H	2.447300	3.631400	5.049300
H	0.916500	4.518100	5.054600
H	2.126600	4.870000	3.814100
C	-0.105000	3.713200	2.689900
H	0.327900	4.495700	2.055700
H	-0.827900	4.185800	3.367200

H	-0.634500	3.004800	2.050300
C	0.363600	1.945600	4.440700
H	-0.163200	1.187300	3.859500
H	-0.356000	2.421100	5.118400
H	1.129400	1.452000	5.051800
C	2.848500	-0.787000	-1.107600
C	3.803800	-1.738400	-0.712900
H	3.944100	-1.964800	0.337200
C	4.550300	-2.382200	-1.690700
C	4.399000	-2.130800	-3.050200
H	4.990300	-2.647400	-3.794700
C	3.446500	-1.178500	-3.400700
C	2.672400	-0.499300	-2.470800
H	1.946600	0.248200	-2.764800
C	0.482300	-2.010800	2.537900
H	0.560900	-1.013300	2.949900
C	0.638400	-3.152000	3.311500
H	0.842200	-3.054900	4.372400
C	0.527300	-4.403700	2.704000
H	0.641800	-5.315000	3.281900
C	0.268400	-4.463900	1.340400
H	0.183300	-5.424700	0.845900
C	0.121600	-3.282800	0.607200
C	-0.144000	-3.229700	-0.833600
C	-0.300700	-4.353500	-1.650100
H	-0.224200	-5.348000	-1.226100
C	-0.558400	-4.192600	-3.005800
H	-0.680700	-5.058800	-3.647900
C	-0.658800	-2.899400	-3.521200
H	-0.861800	-2.724300	-4.572200
C	-0.493200	-1.818400	-2.667200
H	-0.564600	-0.792900	-3.005800
C	-2.551500	0.817300	-0.666300
C	-3.906200	1.227300	-0.686100
H	-4.608000	0.741500	-0.020600
C	-4.313700	2.241400	-1.532600
C	-3.338600	2.857000	-2.364200
H	-3.669000	3.655600	-3.016500
C	-1.992000	2.514300	-2.381900
C	-1.582000	1.460100	-1.511300
C	-0.982500	3.248700	-3.282900
C	-0.348000	2.254400	-4.286000
H	-1.115800	1.807500	-4.929700
H	0.176500	1.454800	-3.760000
H	0.373200	2.773300	-4.929200
C	0.127700	3.893500	-2.415600

H	0.852600	4.409200	-3.058500
H	0.654000	3.140300	-1.826700
H	-0.302200	4.632100	-1.728800
C	-1.649500	4.372100	-4.100200
H	-2.430700	3.989000	-4.767400
H	-0.892200	4.860900	-4.723500
H	-2.091600	5.139000	-3.453600
C	-5.769200	2.732200	-1.597800
C	-5.827100	4.235000	-1.228400
H	-6.861400	4.597500	-1.274800
H	-5.227100	4.845700	-1.910900
H	-5.451100	4.399500	-0.212300
C	-6.317900	2.537900	-3.032800
H	-6.307800	1.478100	-3.312400
H	-5.726100	3.086100	-3.773300
H	-7.351900	2.898900	-3.096200
C	-6.689300	1.967100	-0.627600
H	-6.373200	2.091300	0.414300
H	-6.716600	0.895000	-0.853400
H	-7.712700	2.350400	-0.712000
C	-2.854200	-0.849200	1.051200
C	-3.812700	-1.764700	0.585600
H	-3.951600	-1.912500	-0.478600
C	-4.563900	-2.475900	1.511600
C	-4.414200	-2.326800	2.886300
H	-5.008900	-2.894800	3.589600
C	-3.458400	-1.407300	3.308000
C	-2.679700	-0.664300	2.432300
H	-1.951400	0.056300	2.782400

Optimised cartesian coordinates of **2a** (DFT/B3LYP/SDD/6-31G(d)) (Singlet closed shell, S = 0)

E(Total)= −2461.81517981 a.u.

Ru	0.004100	-0.455600	-0.005800
Cl	-6.272100	-2.967200	-0.794700
Cl	-3.563000	-3.477800	3.911300
Cl	6.311200	-2.921300	0.817400
Cl	3.545500	-3.583600	-3.836800
O	-0.357000	0.999200	-1.372400
O	0.369000	0.980700	1.377800
N	-2.007000	-0.205100	0.229800
N	-0.349000	-2.063000	-1.268400
N	0.340100	-2.080200	1.236300
N	2.017800	-0.211600	-0.236400
C	-1.508100	1.631300	-1.174000
C	-1.868600	2.828300	-1.857300
C	-3.122500	3.356200	-1.570700
H	-3.410600	4.279100	-2.058300
C	-4.051900	2.770700	-0.670900
C	-3.701100	1.585300	-0.047100
H	-4.373600	1.100500	0.649300
C	-2.441000	0.998500	-0.293700
C	-5.400900	3.467500	-0.426800
C	-6.283600	2.699600	0.576000
H	-6.519000	1.689900	0.220600
H	-7.231600	3.232000	0.713500
H	-5.804000	2.616100	1.557900
C	-6.177500	3.575600	-1.762400
H	-5.614100	4.134600	-2.516700
H	-7.132800	4.091400	-1.606100
H	-6.389000	2.580600	-2.170700
C	-5.158700	4.888200	0.139200
H	-4.626400	4.838700	1.095800
H	-6.115300	5.399300	0.304500
H	-4.563800	5.503000	-0.544000
C	-0.908500	3.501900	-2.854800
C	-1.518700	4.776200	-3.470300
H	-2.443200	4.565000	-4.020700
H	-0.804000	5.212300	-4.177300
H	-1.735200	5.534900	-2.709100
C	0.406300	3.903600	-2.142500
H	0.204900	4.613500	-1.332000

H	1.084500	4.387600	-2.857000
H	0.910100	3.032900	-1.720100
C	-0.590000	2.525200	-4.014600
H	-0.104800	1.622600	-3.637500
H	0.083200	3.005700	-4.735600
H	-1.507400	2.240900	-4.544800
C	-2.959200	-1.144800	0.659300
C	-4.037400	-1.519500	-0.169500
H	-4.157900	-1.057900	-1.141700
C	-4.925100	-2.486400	0.273600
C	-4.813800	-3.116700	1.510600
H	-5.520700	-3.868800	1.834700
C	-3.745900	-2.717100	2.306200
C	-2.826000	-1.752900	1.919900
H	-2.029900	-1.441500	2.582000
C	-0.751100	-1.942100	-2.550400
H	-0.830500	-0.921300	-2.906400
C	-1.030000	-3.042900	-3.347400
H	-1.345600	-2.896900	-4.374800
C	-0.895800	-4.322500	-2.804900
H	-1.103900	-5.203100	-3.403700
C	-0.492300	-4.452300	-1.482400
H	-0.389900	-5.436000	-1.038800
C	-0.225000	-3.307800	-0.724700
C	0.198300	-3.317900	0.680200
C	0.450600	-4.473600	1.425900
H	0.336100	-5.451000	0.971600
C	0.855500	-4.363000	2.749600
H	1.052400	-5.252300	3.339200
C	1.006500	-3.091000	3.305400
H	1.323600	-2.960000	4.334300
C	0.743200	-1.978400	2.519900
H	0.837800	-0.962500	2.886200
C	2.448200	0.994100	0.290100
C	3.702100	1.590500	0.036000
H	4.372500	1.112500	-0.666900
C	4.048700	2.778200	0.658500
C	3.121300	3.355300	1.565200
H	3.405300	4.280200	2.051400
C	1.873400	2.817400	1.859700
C	1.516800	1.619300	1.176500
C	0.914800	3.483800	2.863800
C	0.604700	2.503900	4.023300
H	1.524600	2.227800	4.553500
H	0.127900	1.597200	3.646300
H	-0.072500	2.978700	4.744400

C	-0.404200	3.880900	2.157000
H	-1.079600	4.366300	2.873000
H	-0.908400	3.007500	1.740100
H	-0.208200	4.587700	1.342400
C	1.522400	4.758900	3.480300
H	2.451900	4.550100	4.023000
H	0.810400	5.188100	4.194200
H	1.729200	5.522000	2.720900
C	5.389200	3.487500	0.403100
C	5.128100	4.903400	-0.166500
H	6.078300	5.419900	-0.350800
H	4.541200	5.517700	0.524100
H	4.579500	4.845500	-1.113300
C	6.173200	3.609600	1.733200
H	6.394300	2.619000	2.146900
H	5.610800	4.170100	2.487000
H	7.124000	4.131000	1.567400
C	6.273400	2.724700	-0.602200
H	5.789800	2.635600	-1.581600
H	6.518200	1.717600	-0.246000
H	7.216500	3.264300	-0.745300
C	2.970900	-1.156800	-0.647800
C	4.062200	-1.503000	0.177800
H	4.192800	-1.013600	1.134800
C	4.948400	-2.478600	-0.247700
C	4.825200	-3.146700	-1.463800
H	5.531400	-3.905300	-1.774000
C	3.745700	-2.774900	-2.256700
C	2.826300	-1.803400	-1.888200
H	2.022700	-1.514900	-2.551400

Optimised cartesian coordinates of **2a** (DFT/B3LYP/SDD/6-31G(d)) (Singlet BS(1,1), S = 0)

E(Total)= −2461.81929526 a.u.

Ru	0.000300	-0.470900	-0.001100
Cl	6.372700	-2.881500	0.691600
Cl	3.418600	-3.642200	-3.829000
Cl	-6.369300	-2.887500	-0.688500
Cl	-3.413500	-3.640200	3.832300
O	0.343800	0.989400	1.366100
O	-0.344500	0.990000	-1.367400
N	2.014600	-0.209600	-0.231600
N	0.370600	-2.069100	1.236400
N	-0.370500	-2.068500	-1.239400
N	-2.013700	-0.210400	0.230500
C	1.493300	1.628400	1.173900
C	1.844200	2.830800	1.866200
C	3.095000	3.379500	1.574100
H	3.372700	4.311200	2.061900
C	4.032700	2.807000	0.665800
C	3.697100	1.609700	0.039300
H	4.375200	1.132000	-0.663300
C	2.441600	1.003300	0.291500
C	5.367600	3.530900	0.410100
C	6.268200	2.765900	-0.584400
H	6.520500	1.761700	-0.215100
H	7.209100	3.316200	-0.726000
H	5.790300	2.662600	-1.568800
C	6.143600	3.679200	1.746500
H	5.569400	4.249400	2.489100
H	7.093200	4.207900	1.576600
H	6.370800	2.694400	2.177800
C	5.089000	4.941100	-0.175500
H	4.548400	4.866600	-1.129100
H	6.036100	5.471900	-0.355200
H	4.484700	5.551600	0.508800
C	0.875800	3.480300	2.874000
C	1.468000	4.760100	3.505500
H	2.399600	4.556400	4.053200
H	0.744200	5.175700	4.220700
H	1.670900	5.533800	2.750900
C	-0.452600	3.868500	2.171600
H	-0.269500	4.598400	1.370800
H	-1.137100	4.327100	2.901700

H	-0.942900	2.992300	1.736100
C	0.575200	2.482100	4.025200
H	0.106600	1.570900	3.637500
H	-0.110200	2.944400	4.751400
H	1.500000	2.209900	4.554800
C	2.961800	-1.158000	-0.661100
C	4.091600	-1.482700	0.129000
H	4.255600	-0.975800	1.075600
C	4.974100	-2.466400	-0.314600
C	4.795200	-3.156200	-1.521500
H	5.495200	-3.917700	-1.849300
C	3.674900	-2.810500	-2.285100
C	2.763700	-1.831800	-1.886300
H	1.923200	-1.561400	-2.516100
C	0.822300	-1.952300	2.513400
H	0.905300	-0.930000	2.873300
C	1.142000	-3.058500	3.295200
H	1.496600	-2.910700	4.312500
C	0.998400	-4.345300	2.751700
H	1.240500	-5.228600	3.338500
C	0.543000	-4.473200	1.439600
H	0.434900	-5.457300	0.990400
C	0.234900	-3.325300	0.691600
C	-0.235700	-3.325000	-0.694900
C	-0.544600	-4.472400	-1.443200
H	-0.437200	-5.456700	-0.994100
C	-0.999900	-4.344000	-2.755200
H	-1.242700	-5.226900	-3.342200
C	-1.142600	-3.057000	-3.298400
H	-1.497000	-2.908700	-4.315700
C	-0.822100	-1.951100	-2.516400
H	-0.904400	-0.928700	-2.876000
C	-2.441700	1.002500	-0.291500
C	-3.697500	1.608100	-0.038600
H	-4.374900	1.129800	0.664200
C	-4.034200	2.805000	-0.665000
C	-3.097400	3.378400	-1.573700
H	-3.376100	4.309800	-2.061300
C	-1.846200	2.830800	-1.866300
C	-1.494200	1.628400	-1.174400
C	-0.879000	3.481300	-2.874600
C	-0.578600	2.483600	-4.026400
H	-1.503700	2.209700	-4.554400
H	-0.107600	1.573200	-3.639400
H	0.104900	2.947000	-4.753700
C	0.449700	3.870600	-2.173400

H	1.133300	4.329300	-2.904200
H	0.940800	2.994900	-1.737800
H	0.266700	4.600700	-1.372700
C	-1.472900	4.760600	-3.505300
H	-2.406000	4.556400	-4.050400
H	-0.751100	5.175700	-4.222800
H	-1.673800	5.534800	-2.750800
C	-5.369700	3.527800	-0.409000
C	-5.092200	4.938500	0.175900
H	-6.039700	5.468400	0.355600
H	-4.488700	5.549300	-0.508800
H	-4.551400	4.865000	1.129400
C	-6.146300	3.674800	-1.745200
H	-6.372900	2.689600	-2.175800
H	-5.572700	4.244900	-2.488300
H	-7.096300	4.202900	-1.575400
C	-6.269200	2.762400	0.586200
H	-5.790800	2.660100	1.570500
H	-6.520800	1.757900	0.217500
H	-7.210500	3.312000	0.727800
C	-2.960100	-1.159000	0.661900
C	-4.089500	-1.485700	-0.127900
H	-4.254000	-0.980100	-1.075100
C	-4.971000	-2.469800	0.317000
C	-4.791200	-3.157800	1.524700
H	-5.490300	-3.919700	1.853500
C	-3.671100	-2.810200	2.287700
C	-2.760900	-1.831100	1.887700
H	-1.920200	-1.559300	2.516700

Optimised cartesian coordinates of **2a**$^{+}$ (DFT/UB3LYP/SDD/6-31G(d))

E(Total)= −2461.55663391 a.u.

Ru	0.548500	-0.547600	-0.018600
O	0.548500	1.502100	-0.018600
O	-1.499800	-0.488400	-0.018600
N	0.602000	-0.148400	-2.040300
N	2.612500	-0.793700	0.011700
N	0.735900	-2.616600	-0.058100
N	0.148300	-0.594500	2.003600
C	0.280300	2.019400	-1.178800
C	0.040300	3.403300	-1.363700
C	-0.207900	3.881700	-2.631700
C	-0.215900	3.017300	-3.765400
C	0.040600	1.674800	-3.631200
C	0.303900	1.137100	-2.334200
C	0.950600	-1.049700	-3.084500
C	2.065400	-0.795800	-3.901100
C	2.422000	-1.705400	-4.896300
C	1.666900	-2.863400	-5.096700
C	0.551200	-3.110300	-4.292300
C	0.197400	-2.215700	-3.282800
C	3.499300	0.220200	0.010100
C	4.871500	0.006800	-0.025400
C	5.347500	-1.304700	-0.059400
C	4.434000	-2.353900	-0.059600
C	3.063600	-2.078500	-0.025800
C	2.007400	-3.104600	-0.031600
C	2.243600	-4.482600	-0.008100
C	1.168600	-5.365600	-0.007600
C	-0.128800	-4.851900	-0.030400
C	-0.302900	-3.474000	-0.056000
C	-1.127400	-0.254000	2.296700
C	-1.655900	0.028500	3.593300
C	-2.988800	0.331700	3.727200
C	-3.852400	0.353100	2.593300
C	-3.382500	0.087400	1.325600
C	-2.007900	-0.201100	1.141400
C	1.033200	-0.983000	3.046900
C	0.730800	-2.085500	3.864400
C	1.624900	-2.482500	4.858000
C	2.815800	-1.779800	5.057400
C	3.111000	-0.675800	4.253100
C	2.232000	-0.282600	3.244700
C	0.038600	4.327600	-0.131900

C	-0.103600	5.791400	-0.588700
C	1.360200	4.156800	0.639900
C	-1.142600	3.958900	0.784900
C	-0.537000	3.604600	-5.152300
C	0.774800	3.864100	-5.916100
C	-1.303500	4.929600	-4.983800
C	-1.403300	2.607500	-5.944000
C	-4.305500	0.121200	0.093400
C	-5.767100	0.281600	0.551100
C	-3.916300	1.308400	-0.807100
C	-4.156100	-1.192500	-0.696200
C	-3.564300	0.675400	5.113600
C	-2.494800	1.406100	5.946600
C	-3.978000	-0.621600	5.833600
C	-4.795500	1.585300	4.947100
Cl	3.825800	-1.379000	-5.906400
Cl	-1.227800	-2.496500	-2.288900
Cl	4.593400	0.235800	4.516000
Cl	1.237900	-3.871300	5.867600
H	-0.415200	4.938800	-2.775100
H	0.019900	1.012300	-4.489100
H	2.648000	0.107000	-3.744900
H	1.941400	-3.564400	-5.879000
H	-0.051800	-3.000000	-4.455400
H	3.067600	1.214600	0.042300
H	5.547900	0.854900	-0.026700
H	6.413400	-1.507600	-0.087900
H	4.785000	-3.378500	-0.093000
H	3.257900	-4.863000	0.016600
H	1.341000	-6.437000	0.012900
H	-0.996000	-5.503700	-0.028100
H	-1.284700	-3.013800	-0.079000
H	-0.992900	0.028300	4.451100
H	-4.901800	0.597300	2.736100
H	-0.196400	-2.628400	3.708500
H	3.504700	-2.085700	5.838700
H	2.442700	0.588200	2.633500
H	-1.043700	5.921000	-1.082900
H	-0.056500	6.437000	0.263200
H	0.690600	6.033100	-1.263700
H	1.203400	3.508600	1.476700
H	2.098700	3.731500	-0.007100
H	1.696800	5.111500	0.986400
H	-1.843000	3.360200	0.240900
H	-0.781300	3.407700	1.627900
H	-1.624200	4.852600	1.123000

H	1.094400	2.961200	-6.393100
H	0.613400	4.620300	-6.655700
H	1.528200	4.191100	-5.230300
H	-2.135900	4.779300	-4.328400
H	-0.651100	5.668700	-4.567900
H	-1.656200	5.261500	-5.937900
H	-0.799900	1.781400	-6.257600
H	-2.197900	2.252700	-5.321400
H	-1.814100	3.095600	-6.803000
H	-6.413400	0.249000	-0.301100
H	-6.020300	-0.513200	1.221300
H	-5.883300	1.220400	1.051100
H	-3.323200	2.001100	-0.247400
H	-3.353300	0.951600	-1.644100
H	-4.802100	1.797200	-1.155400
H	-3.474700	-1.045300	-1.507900
H	-3.779800	-1.956900	-0.048800
H	-5.110000	-1.488200	-1.080400
H	-1.751300	0.705900	6.265700
H	-2.035800	2.166400	5.349700
H	-2.954100	1.853700	6.803000
H	-3.103500	-1.132400	6.178900
H	-4.604100	-0.382300	6.667700
H	-4.513900	-1.251200	5.154400
H	-4.541300	2.419400	4.327000
H	-5.589600	1.031200	4.491800
H	-5.111000	1.937600	5.907000

Optimised cartesian coordinates of **2a**$^{2+}$ (DFT/B3LYP/SDD/6-31G(d))

E(Total)= −2461.26345494 a.u.

Ru	0.000300	-0.334000	-0.000400
O	0.430100	1.119200	1.412400
O	-0.428800	1.123700	-1.408700
N	2.051500	-0.115400	-0.189900
N	0.266100	-1.949400	1.286000
N	-0.265900	-1.945900	-1.291000
N	-2.050500	-0.115200	0.189900
C	1.651100	1.475600	1.489800
C	2.114200	2.479400	2.392200
C	3.441200	2.810500	2.380700
H	3.809000	3.579800	3.053500
C	4.380400	2.183500	1.479100
C	3.993800	1.209900	0.608100
H	4.697200	0.758700	-0.081000
C	2.612500	0.798400	0.593600
C	2.864300	-0.880300	-1.084000
C	3.861600	-1.732000	-0.582500
H	4.017700	-1.813300	0.489200
C	4.630100	-2.484600	-1.470700
C	4.428300	-2.370500	-2.848500
H	5.041400	-2.944300	-3.536400
C	3.442200	-1.509600	-3.341300
C	2.643800	-0.776700	-2.464700
H	1.893900	-0.086400	-2.837000
C	0.563700	-1.851500	2.596100
H	0.630500	-0.846200	2.994300
C	0.770700	-2.967100	3.399700
H	1.010600	-2.836600	4.449300
C	0.661500	-4.234600	2.828400
H	0.815400	-5.128200	3.424700
C	0.352400	-4.339900	1.474400
H	0.268600	-5.317200	1.014400
C	0.160300	-3.183200	0.715000
C	-0.159400	-3.181200	-0.723500
C	-0.351800	-4.335900	-1.486000
H	-0.267700	-5.314400	-1.028700
C	-0.662000	-4.226900	-2.839400
H	-0.816300	-5.118900	-3.438100
C	-0.772400	-2.957900	-3.407000
H	-1.013500	-2.824500	-4.456000
C	-0.565100	-1.844400	-2.600500
H	-0.633100	-0.838000	-2.995700

C	-2.611200	0.800900	-0.590700
C	-3.992800	1.211000	-0.604700
H	-4.696200	0.756700	0.082400
C	-4.379600	2.187200	-1.472700
C	-3.440200	2.817700	-2.371900
H	-3.808200	3.588700	-3.042500
C	-2.113100	2.487100	-2.384200
C	-1.649700	1.480800	-1.484800
C	-2.864000	-0.882200	1.081400
C	-3.864600	-1.728000	0.576800
H	-4.023000	-1.802500	-0.495100
C	-4.634200	-2.482900	1.462100
C	-4.429900	-2.376900	2.840300
H	-5.043800	-2.952400	3.526000
C	-3.440700	-1.521500	3.336200
C	-2.641500	-0.786100	2.462400
H	-1.888900	-0.100100	2.837200
Cl	-3.199500	-1.351500	5.132100
Cl	-5.921200	-3.592100	0.809600
Cl	3.204200	-1.329400	-5.136600
Cl	5.912300	-3.601800	-0.822300
C	-5.845400	2.658900	-1.494300
C	-6.313100	2.947300	-0.055700
H	-6.591100	2.029800	0.419600
H	-5.517300	3.406300	0.492800
H	-7.155900	3.606100	-0.080000
C	-5.959300	3.942200	-2.338100
H	-5.695100	3.726700	-3.352400
H	-6.965100	4.305300	-2.300900
H	-5.296800	4.686000	-1.947300
C	-6.729600	1.559000	-2.110800
H	-6.226800	1.126000	-2.950300
H	-6.919000	0.801800	-1.379000
H	-7.657200	1.985100	-2.431600
C	-1.095000	3.174500	-3.313000
C	-1.803900	4.270600	-4.130100
H	-2.575900	3.828900	-4.725000
H	-2.233900	4.989700	-3.464600
H	-1.094600	4.754700	-4.768400
C	0.025100	3.808300	-2.467200
H	-0.303400	3.902500	-1.453300
H	0.895100	3.186500	-2.504000
H	0.261900	4.776300	-2.856800
C	-0.488000	2.132100	-4.270400
H	0.490400	1.863200	-3.930900
H	-1.110100	1.261800	-4.290900

H	-0.422600	2.547100	-5.254400
C	1.096000	3.163700	3.323100
C	0.466000	2.112800	4.255900
H	-0.524400	1.886100	3.920600
H	1.059600	1.222600	4.242600
H	0.425300	2.499400	5.252800
C	-0.007400	3.827000	2.477900
H	0.343900	3.963400	1.476400
H	-0.875000	3.200900	2.469300
H	-0.257600	4.777500	2.900600
C	1.811000	4.235800	4.166300
H	1.101900	4.717300	4.806700
H	2.571700	3.773700	4.760100
H	2.256100	4.961200	3.517800
C	5.845900	2.656200	1.501500
C	5.928800	4.039900	2.172300
H	5.695100	3.946700	3.212300
H	6.918900	4.430600	2.062900
H	5.230000	4.703900	1.707900
C	6.698100	1.648900	2.295700
H	6.955900	0.824100	1.664600
H	7.591100	2.128900	2.637900
H	6.139500	1.293700	3.136300
C	6.376300	2.752400	0.059000
H	6.549200	1.768300	-0.323900
H	5.655100	3.251800	-0.553700
H	7.293200	3.304000	0.052100

Optimised cartesian coordinates of **2a**$^{-}$ (DFT/B3LYP/SDD/6-31G(d))

E(Total)= −2461.86842808 a.u

Ru	-0.021100	-0.432900	0.169400
Cl	6.338300	-3.018800	0.981700
Cl	2.912900	-4.601600	-3.158700
Cl	-6.355000	-2.324800	-1.648800
Cl	-3.536500	-4.747600	2.544300
O	0.557700	1.157700	1.417200
N	2.011800	-0.268200	-0.302200
C	1.715900	1.746800	0.984100
C	2.168700	3.016200	1.464500
C	3.368800	3.522800	0.928300
H	3.707900	4.499900	1.256000
C	4.150500	2.833400	-0.039600
C	3.714500	1.565300	-0.463400
H	4.281600	0.992300	-1.192800
C	2.520300	1.010200	0.046700
C	5.406400	3.524000	-0.634000
C	6.261900	2.538900	-1.494800
H	6.537500	1.655500	-0.898500
H	7.179900	3.049400	-1.828100
H	5.701200	2.208700	-2.383300
C	6.327600	4.061900	0.528900
H	5.861100	4.923700	1.031000
H	7.298500	4.379500	0.113200
H	6.488900	3.263900	1.270300
C	4.966200	4.723700	-1.535600
H	4.485100	4.347100	-2.452200
H	5.847200	5.330700	-1.811700
H	4.246700	5.358400	-0.997300
C	1.361600	3.777100	2.549600
C	2.042900	5.126500	2.950300
H	3.075700	4.954400	3.293300
H	1.465600	5.584800	3.768800
H	2.060500	5.820200	2.093600
C	-0.081400	4.099000	2.032400
H	-0.023900	4.718600	1.124900
H	-0.635000	4.649800	2.812900
H	-0.616000	3.172100	1.791700
C	1.269100	2.891500	3.842500
H	0.747100	1.954400	3.610600
H	0.713200	3.435500	4.626000
H	2.283300	2.661000	4.211600
C	2.872500	-1.343600	-0.584800

C	4.047000	-1.584500	0.195100
H	4.319000	-0.888700	0.986600
C	4.818900	-2.711600	-0.058100
C	4.501400	-3.657800	-1.046700
H	5.113800	-4.539300	-1.217400
C	3.348500	-3.396200	-1.800000
C	2.542800	-2.274900	-1.613800
H	1.684700	-2.093200	-2.250900
O	-0.489000	1.009800	-1.305700
N	-2.069800	-0.116100	0.520500
C	-2.441800	1.188500	0.064900
C	-3.577100	1.883900	0.523000
H	-4.181200	1.427700	1.302800
C	-3.901900	3.144200	-0.010300
C	-3.075100	3.659900	-1.047600
H	-3.334600	4.622000	-1.478300
C	-1.931000	3.001500	-1.537400
C	-1.579500	1.749000	-0.933200
C	-1.088200	3.568700	-2.711800
C	-1.096300	2.531500	-3.889500
H	-2.133400	2.341800	-4.215400
H	-0.644700	1.589300	-3.552800
H	-0.516100	2.931200	-4.739400
C	0.387400	3.826000	-2.253000
H	1.004600	4.090700	-3.128800
H	0.800900	2.927800	-1.780400
H	0.414700	4.655600	-1.529300
C	-1.663800	4.913100	-3.261700
H	-2.683300	4.767400	-3.656200
H	-1.011800	5.267400	-4.075800
H	-1.691900	5.679300	-2.469900
C	-5.092100	3.994400	0.511500
C	-4.547600	5.311600	1.160300
H	-5.391200	5.957900	1.460900
H	-3.913800	5.858100	0.445800
H	-3.943300	5.065400	2.047700
C	-6.052400	4.355900	-0.676200
H	-6.403200	3.431800	-1.162000
H	-5.529800	4.972300	-1.422600
H	-6.921900	4.919200	-0.294900
C	-5.930200	3.229300	1.583000
H	-5.306800	2.976600	2.453600
H	-6.340400	2.302000	1.154800
H	-6.763400	3.869800	1.916700
C	-3.038700	-1.134100	0.558700
C	-4.118300	-1.177200	-0.379300

H	-4.247500	-0.357900	-1.083200
C	-4.975500	-2.269100	-0.390200
C	-4.830400	-3.373800	0.467800
H	-5.500500	-4.228100	0.426400
C	-3.766700	-3.306200	1.377800
C	-2.891300	-2.227100	1.467300
H	-2.112600	-2.202800	2.221800
N	0.395500	-1.932900	1.542100
N	-0.519400	-2.150300	-0.912400
C	0.879900	-1.704400	2.805500
H	1.006400	-0.660500	3.083400
C	1.190900	-2.749300	3.674100
H	1.575300	-2.528700	4.668900
C	1.007200	-4.087700	3.244000
H	1.247100	-4.919900	3.906000
C	0.514500	-4.328300	1.957400
H	0.369400	-5.349000	1.613400
C	0.209600	-3.244800	1.105100
C	-0.343300	-3.364900	-0.245800
C	-0.662800	-4.579300	-0.887800
H	-0.514900	-5.523900	-0.369600
C	-1.182800	-4.568100	-2.187500
H	-1.432300	-5.504500	-2.686100
C	-1.382100	-3.330900	-2.838600
H	-1.790500	-3.286800	-3.847500
C	-1.045700	-2.147500	-2.173700
H	-1.188400	-1.173200	-2.636100

Table S19 Optimised cartesian coordinates of **2b (**DFT/UB3LYP/SDD/6-31G(d))

(Triplet state, S=1)

E(Total)= −2461.81009514 a.u.

Ru	-0.094600	-0.236300	0.932600
Cl	6.457700	-0.526400	1.714300
Cl	3.906900	-4.307300	-1.211300
Cl	1.553300	-1.323000	-4.730900
Cl	-2.954700	-4.192800	-3.848900
O	-0.260300	1.781600	0.679800
O	-1.876200	-0.205300	1.942000
N	1.652000	0.174200	-0.037200
N	-1.415800	-0.487800	-0.608500
C	0.698400	2.343500	-0.045000
C	0.722100	3.740900	-0.373200
C	1.807600	4.185900	-1.118500
H	1.837400	5.231900	-1.384200
C	2.879000	3.368400	-1.562800
C	2.847400	2.026200	-1.220000
H	3.630500	1.352600	-1.548400
C	1.786600	1.497100	-0.449800
C	4.051500	3.934200	-2.394900
C	5.376000	3.731800	-1.620300
H	6.221300	4.130200	-2.195000
H	5.578200	2.675000	-1.423400
H	5.349900	4.251100	-0.655600
C	3.903500	5.440900	-2.683700
H	3.003200	5.664000	-3.265900
H	4.763200	5.786400	-3.268000
H	3.874200	6.037600	-1.765700
C	4.134900	3.198000	-3.752700
H	3.210900	3.327700	-4.326900
H	4.299200	2.124300	-3.626700
H	4.965000	3.592500	-4.351600
C	-0.395500	4.710700	0.076400
C	-0.125400	6.157500	-0.384400
H	0.808200	6.560600	0.023400
H	-0.938500	6.802100	-0.033000
H	-0.092100	6.245700	-1.475500
C	-1.755600	4.281600	-0.527100
H	-1.714000	4.299000	-1.622300
H	-2.542100	4.977800	-0.210000
H	-2.044100	3.278300	-0.214100
C	-0.492100	4.738700	1.622600

H	-0.763100	3.762800	2.027200
H	-1.258400	5.457400	1.938300
H	0.461100	5.050700	2.066400
C	2.799900	-0.633000	0.015700
C	3.950500	-0.210300	0.712500
H	3.971800	0.767500	1.178000
C	5.045200	-1.058000	0.818900
C	5.057900	-2.329000	0.243200
H	5.920300	-2.978400	0.329600
C	3.916700	-2.727800	-0.451800
C	2.796300	-1.912000	-0.566800
H	1.932500	-2.247500	-1.124700
C	-2.715300	-0.134400	-0.266900
C	-3.782500	0.118800	-1.156200
H	-3.580500	0.075100	-2.218500
C	-5.042400	0.446000	-0.688500
C	-5.227000	0.505800	0.720500
H	-6.217600	0.747500	1.081600
C	-4.227700	0.309400	1.659900
C	-2.917700	0.003600	1.154000
C	-4.506500	0.420000	3.175100
C	-5.986700	0.734900	3.470500
H	-6.130300	0.798200	4.554800
H	-6.661000	-0.045100	3.100000
H	-6.301900	1.693800	3.045100
C	-4.173400	-0.920400	3.876300
H	-3.125500	-1.193500	3.746900
H	-4.791100	-1.731800	3.474100
H	-4.378500	-0.844500	4.951500
C	-3.662800	1.564700	3.788700
H	-2.593700	1.392000	3.660500
H	-3.870800	1.650400	4.862600
H	-3.911800	2.523700	3.319800
C	-6.228200	0.757100	-1.622200
C	-5.837800	0.683900	-3.109500
H	-6.711200	0.908900	-3.731200
H	-5.484200	-0.312100	-3.394300
H	-5.058700	1.409600	-3.365200
C	-6.756600	2.183300	-1.336400
H	-5.972800	2.930500	-1.503200
H	-7.107600	2.294400	-0.306100
H	-7.598400	2.420000	-1.998500
C	-7.359200	-0.270700	-1.377000
H	-7.718700	-0.249000	-0.343800
H	-7.014500	-1.288900	-1.588200
H	-8.214800	-0.061200	-2.030900

C	-1.221400	-1.165900	-1.808900
C	-0.078500	-0.917900	-2.597100
H	0.611500	-0.138400	-2.304800
C	0.140600	-1.660400	-3.751400
C	-0.727200	-2.669800	-4.170600
H	-0.535100	-3.239800	-5.071000
C	-1.851300	-2.910600	-3.379300
C	-2.112400	-2.184400	-2.226700
H	-2.988000	-2.412600	-1.631700
N	0.935600	-0.130600	2.734900
N	0.174100	-2.246100	1.400800
C	1.233200	1.008800	3.401700
H	0.903800	1.923300	2.923800
C	1.918800	1.026600	4.605700
H	2.133400	1.977300	5.084600
C	2.321600	-0.186100	5.169900
H	2.867600	-0.213000	6.108700
C	2.001500	-1.364600	4.510000
H	2.291200	-2.316000	4.940000
C	1.302700	-1.323300	3.297100
C	0.889500	-2.509600	2.545200
C	1.178300	-3.819800	2.945700
H	1.764800	-3.997900	3.839400
C	0.715500	-4.896400	2.202600
H	0.940100	-5.914600	2.507300
C	-0.042800	-4.633800	1.060000
H	-0.439600	-5.432500	0.440300
C	-0.283300	-3.317000	0.702500
H	-0.854300	-3.082200	-0.185800

Optimised cartesian coordinates of **2b (**DFT/B3LYP/SDD/6-31G(d)) (Singlet closed shell, S = 0)

E(Total)= −2461.81285134 a.u.

Ru	0.004900	-0.610600	-0.848100
Cl	-6.635700	0.539900	-1.699100
Cl	-4.775100	-3.449000	1.686900
Cl	-1.910600	-0.210200	4.856300
Cl	2.706500	-3.290400	5.010000
O	0.492300	1.328000	-1.214500
O	1.728300	-1.141100	-1.773800
N	-1.632800	0.332400	-0.102600
N	1.276200	-0.594200	0.729000
C	-0.261200	2.236700	-0.544000
C	0.028600	3.634100	-0.487400
C	-0.875000	4.443000	0.225700
H	-0.658100	5.499600	0.301400
C	-2.047900	3.952200	0.864000
C	-2.327800	2.581300	0.766500
H	-3.205600	2.163200	1.249600
C	-1.453600	1.720600	0.062700
C	-2.996700	4.870100	1.675000
C	-4.429200	4.811500	1.063200
H	-5.116600	5.445700	1.639600
H	-4.830400	3.791000	1.068700
H	-4.423700	5.166200	0.024100
C	-2.535700	6.349900	1.676300
H	-1.546600	6.466000	2.137900
H	-3.246400	6.954500	2.254500
H	-2.493700	6.765700	0.661200
C	-3.051600	4.380800	3.153500
H	-2.056700	4.422700	3.615000
H	-3.409800	3.347000	3.225600
H	-3.730600	5.014900	3.740200
C	1.295100	4.215700	-1.157700
C	1.393900	5.754000	-0.988100
H	0.538300	6.274100	-1.439400
H	2.303400	6.112200	-1.487900
H	1.458700	6.046000	0.068300
C	2.563900	3.578800	-0.516400
H	2.612500	3.811600	0.556000
H	3.468000	3.979800	-0.996200
H	2.562700	2.493200	-0.636500
C	1.274200	3.904400	-2.684400

H	1.272300	2.825000	-2.856200
H	2.164000	4.332600	-3.166600
H	0.385300	4.343800	-3.158800
C	-2.948000	-0.205100	-0.043200
C	-4.018200	0.385900	-0.769200
H	-3.846300	1.285100	-1.350100
C	-5.278100	-0.212700	-0.734300
C	-5.552800	-1.382000	-0.004700
H	-6.539700	-1.828500	0.008700
C	-4.479200	-1.933000	0.708700
C	-3.197500	-1.377000	0.711600
H	-2.405500	-1.809100	1.308100
C	2.594400	-0.379800	0.288100
C	3.675500	0.067300	1.092500
H	3.488100	0.311200	2.131100
C	4.945700	0.237100	0.538200
C	5.128100	-0.071700	-0.846700
H	6.117800	0.059900	-1.268400
C	4.102800	-0.515000	-1.689900
C	2.803800	-0.662800	-1.104400
C	4.339000	-0.827700	-3.184900
C	5.811200	-0.582000	-3.604100
H	5.926700	-0.816100	-4.670500
H	6.508700	-1.221000	-3.046400
H	6.108400	0.465000	-3.458200
C	4.001100	-2.324200	-3.463500
H	2.960500	-2.539600	-3.206200
H	4.651600	-2.984300	-2.873300
H	4.157700	-2.552500	-4.527300
C	3.432600	0.086800	-4.062700
H	2.377300	-0.077800	-3.831500
H	3.600600	-0.130700	-5.127100
H	3.665000	1.145800	-3.887400
C	6.149100	0.760000	1.357700
C	5.778800	1.045000	2.835400
H	6.664600	1.406600	3.373200
H	5.424300	0.140900	3.347100
H	5.001300	1.815300	2.917100
C	6.672900	2.084700	0.725400
H	5.888300	2.852200	0.724800
H	7.000700	1.938200	-0.310800
H	7.528700	2.467100	1.298400
C	7.289800	-0.301600	1.340200
H	7.621200	-0.526500	0.319500
H	6.956500	-1.241100	1.800000
H	8.158900	0.066400	1.902500

C	1.025100	-0.941100	2.082000
C	-0.146200	-0.466900	2.726100
H	-0.818400	0.192600	2.194800
C	-0.404900	-0.847700	4.043500
C	0.436900	-1.695800	4.781900
H	0.213600	-1.978000	5.803500
C	1.581100	-2.159700	4.115400
C	1.892000	-1.813100	2.798500
H	2.782200	-2.207100	2.321700
N	-0.954900	-0.868000	-2.671500
N	-0.637500	-2.595800	-0.730500
C	-0.992600	0.100600	-3.625400
H	-0.530700	1.042400	-3.350900
C	-1.585200	-0.121000	-4.873600
H	-1.599500	0.674500	-5.611200
C	-2.153400	-1.383500	-5.145700
H	-2.620000	-1.583900	-6.105800
C	-2.102800	-2.382600	-4.163300
H	-2.523100	-3.362400	-4.360900
C	-1.494000	-2.102600	-2.923600
C	-1.338700	-3.066600	-1.822900
C	-1.842600	-4.381100	-1.856400
H	-2.409500	-4.722900	-2.715100
C	-1.611700	-5.243900	-0.777100
H	-2.002500	-6.256800	-0.786400
C	-0.861100	-4.769300	0.317100
H	-0.643500	-5.402300	1.171000
C	-0.393600	-3.451700	0.302400
H	0.186000	-3.058700	1.126300

Optimised cartesian coordinates of **2b**$^{+}$ **(**DFT/UB3LYP/SDD/6-31G(d))

E(Total)= −2461.61750934 a.u.

Ru	-0.096100	-1.181400	0.015400
Cl	-6.302500	-1.888000	-1.387600
Cl	-5.206800	1.043600	3.096600
O	0.659600	-0.361100	-1.772700
N	-1.592800	0.124000	-0.545100
C	0.066700	0.739200	-2.134100
C	0.544700	1.605300	-3.163400
C	-0.208000	2.723200	-3.441700
H	0.155600	3.404800	-4.204300
C	-1.460300	3.064200	-2.802400
C	-1.957800	2.194600	-1.850500
H	-2.914200	2.378700	-1.361800
C	-1.214100	1.028300	-1.486000
C	-2.217800	4.380700	-3.119500
C	-3.674000	4.050100	-3.578400
H	-4.235300	4.985200	-3.724600
H	-4.195900	3.442700	-2.826300
H	-3.655600	3.491900	-4.526700
C	-1.526200	5.207800	-4.242000
H	-0.488300	5.449900	-3.969200
H	-2.076200	6.147900	-4.387900
H	-1.520400	4.653800	-5.193100
C	-2.276200	5.257200	-1.824200
H	-1.259800	5.510500	-1.486900
H	-2.787500	4.722400	-1.011100
H	-2.824900	6.187500	-2.036000
C	1.852400	1.281900	-3.932600
C	2.207600	2.392300	-4.963000
H	1.429300	2.477500	-5.736800
H	3.158600	2.135800	-5.449200
H	2.317500	3.369200	-4.468400
C	3.053600	1.133800	-2.941800
H	3.205800	2.070500	-2.384000
H	3.966600	0.905900	-3.512800
H	2.865700	0.325200	-2.229700
C	1.665300	-0.059900	-4.718500
H	1.505200	-0.893400	-4.021900
H	2.566100	-0.265600	-5.317200
H	0.799400	0.011100	-5.395400
C	-2.960600	0.018200	-0.114900

C	-3.866400	-0.723300	-0.897700
H	-3.563400	-1.130400	-1.860800
C	-5.167000	-0.917200	-0.423900
C	-5.602000	-0.379500	0.791100
H	-6.622400	-0.528600	1.138200
C	-4.682300	0.357300	1.545500
C	-3.365600	0.557900	1.117600
H	-2.670700	1.133100	1.725100
Cl	-1.628400	4.198700	2.522000
Cl	2.418500	2.225600	5.623100
O	1.656400	-2.326400	0.174300
N	1.221400	0.114600	1.028400
C	2.503500	-0.204000	0.726600
C	3.629700	0.678200	0.829200
H	3.460900	1.685700	1.200100
C	4.887200	0.257500	0.461000
C	5.048300	-1.091900	-0.007200
H	6.052400	-1.406500	-0.281600
C	4.028000	-2.012800	-0.140500
C	2.707300	-1.563900	0.222400
C	4.260200	-3.455900	-0.660600
C	5.751700	-3.696200	-1.034600
H	5.868700	-4.733500	-1.377300
H	6.407500	-3.538300	-0.165000
H	6.070400	-3.020800	-1.843500
C	3.868600	-4.485100	0.450900
H	2.823000	-4.352300	0.756500
H	4.514900	-4.353200	1.332300
H	3.997900	-5.507900	0.064200
C	3.400100	-3.706500	-1.942300
H	2.337200	-3.543800	-1.727500
H	3.541000	-4.743900	-2.283600
H	3.710300	-3.022600	-2.747400
C	6.121400	1.186700	0.509500
C	5.783400	2.595200	1.067300
H	6.703800	3.192200	1.131700
H	5.343900	2.520600	2.073200
H	5.073900	3.117900	0.408800
C	6.704900	1.350300	-0.936500
H	5.977000	1.850400	-1.591500
H	6.950500	0.371500	-1.371400
H	7.622600	1.956100	-0.893000
C	7.218700	0.538300	1.421600
H	7.516600	-0.447800	1.039000
H	6.845200	0.413800	2.449800
H	8.105700	1.188800	1.438900

C	0.962100	1.118400	1.998000
C	-0.075700	2.053900	1.795900
H	-0.664200	2.033200	0.884400
C	-0.327900	3.014500	2.777300
C	0.420700	3.091800	3.958000
H	0.205700	3.846600	4.711500
C	1.451400	2.161100	4.136900
C	1.729000	1.177900	3.187100
H	2.524100	0.455200	3.362300
N	-1.102700	-2.783700	-0.909100
N	-1.162200	-2.029300	1.623100
C	-0.972100	-3.127300	-2.216900
H	-0.274000	-2.517900	-2.789500
C	-1.679900	-4.182100	-2.787200
H	-1.547000	-4.414500	-3.843700
C	-2.554100	-4.924700	-1.982000
H	-3.123600	-5.756000	-2.398100
C	-2.688200	-4.586000	-0.636400
H	-3.354800	-5.159900	0.003700
C	-1.956000	-3.506300	-0.111800
C	-2.028400	-3.052000	1.290100
C	-2.906800	-3.601700	2.238400
H	-3.575600	-4.411100	1.952500
C	-2.921700	-3.112700	3.544200
H	-3.610200	-3.523800	4.282300
C	-2.035000	-2.084700	3.884800
H	-2.000600	-1.672400	4.892900
C	-1.177200	-1.583500	2.909100
H	-0.465200	-0.797200	3.147400

Optimised cartesian coordinates of **2b**$^{2+}$ **(**DFT/B3LYP/sdd/6-31G(d))

E(Total)= −2461.31541499 a.u.

Ru	0.000900	-0.839500	-0.742800
Cl	-6.325500	-0.985200	-2.010400
Cl	-4.917400	-1.738300	3.214900
O	0.544300	1.084000	-1.446600
N	-1.638600	0.339300	-0.270800
C	-0.208000	2.049700	-1.075800
C	0.082800	3.436400	-1.314900
C	-0.884100	4.330700	-0.915700
H	-0.693600	5.384400	-1.084100
C	-2.154900	3.990900	-0.298800
C	-2.435100	2.667700	-0.056700
H	-3.363200	2.362300	0.422100
C	-1.488000	1.660900	-0.425000
C	-3.175900	5.086600	0.081500
C	-4.540300	4.775400	-0.615900
H	-5.280700	5.522100	-0.305100
H	-4.920600	3.783900	-0.342300
H	-4.440000	4.816900	-1.708200
C	-2.725800	6.514100	-0.333200
H	-1.777100	6.793500	0.144000
H	-3.486000	7.235200	-0.014400
H	-2.612100	6.601100	-1.421500
C	-3.376100	5.075800	1.633400
H	-2.435500	5.301300	2.153200
H	-3.737600	4.101300	1.982400
H	-4.116000	5.838200	1.905100
C	1.399900	3.867600	-2.003100
C	1.541600	5.412500	-2.044100
H	0.740900	5.874700	-2.635900
H	2.497700	5.672200	-2.511200
H	1.525100	5.848300	-1.036000
C	2.644500	3.276500	-1.257300
H	2.680800	3.618600	-0.214300
H	3.551300	3.621600	-1.769400
H	2.629900	2.185200	-1.272800
C	1.392500	3.344200	-3.478500
H	1.380700	2.248400	-3.508800
H	2.296100	3.695600	-3.992300
H	0.517500	3.722900	-4.023400
C	-2.941600	-0.202000	0.052300

C	-3.875500	-0.321100	-0.992100
H	-3.642300	0.029000	-1.992600
C	-5.132900	-0.866300	-0.710400
C	-5.471400	-1.308000	0.571800
H	-6.453900	-1.721100	0.777500
C	-4.511500	-1.194600	1.583900
C	-3.241900	-0.652600	1.344500
H	-2.524700	-0.560600	2.152100
Cl	-1.645800	1.333900	4.665500
Cl	2.583700	-1.971600	5.644100
O	1.851300	-1.537600	-1.480700
N	1.367800	-0.462200	0.840600
C	2.634600	-0.376100	0.413800
C	3.729700	0.249000	1.097600
H	3.534900	0.739000	2.046500
C	4.975700	0.257400	0.535300
C	5.187100	-0.434000	-0.723800
H	6.198200	-0.430300	-1.116100
C	4.223200	-1.063800	-1.466200
C	2.863000	-1.011200	-0.922100
C	4.518400	-1.788600	-2.799200
C	6.018700	-1.698600	-3.184300
H	6.177100	-2.241500	-4.122400
H	6.659900	-2.154500	-2.418200
H	6.337300	-0.658800	-3.336100
C	4.144300	-3.302200	-2.662600
H	3.087800	-3.437200	-2.406600
H	4.755400	-3.784200	-1.888100
H	4.336900	-3.804600	-3.618600
C	3.689100	-1.140400	-3.953000
H	2.616600	-1.191900	-3.741700
H	3.886400	-1.680800	-4.887000
H	3.973600	-0.088900	-4.094600
C	6.166600	0.985100	1.174900
C	5.793700	1.674000	2.513100
H	6.686600	2.144200	2.938700
H	5.412600	0.949800	3.245400
H	5.037900	2.455800	2.364700
C	6.704000	2.074300	0.183200
H	5.942600	2.842200	-0.000200
H	6.999200	1.642600	-0.781000
H	7.586000	2.552100	0.626600
C	7.308200	-0.051900	1.459500
H	7.652700	-0.546300	0.543500
H	6.970300	-0.824600	2.161700
H	8.161300	0.477000	1.901700

C	1.105100	-0.366800	2.235600
C	0.008800	0.381500	2.702600
H	-0.599200	0.953300	2.013100
C	-0.265200	0.403100	4.072900
C	0.514700	-0.304500	4.994500
H	0.282600	-0.283000	6.054800
C	1.596100	-1.052600	4.510700
C	1.904000	-1.093000	3.149800
H	2.733100	-1.699600	2.795700
N	-0.955700	-1.539600	-2.494100
N	-0.818300	-2.676700	-0.098400
C	-0.886000	-0.930400	-3.704400
H	-0.313200	-0.007600	-3.733900
C	-1.503400	-1.454800	-4.837000
H	-1.421200	-0.934500	-5.787600
C	-2.221200	-2.651400	-4.720500
H	-2.713900	-3.087700	-5.586000
C	-2.292200	-3.283700	-3.478800
H	-2.833200	-4.218400	-3.379000
C	-1.648200	-2.716000	-2.367100
C	-1.609200	-3.326600	-1.023300
C	-2.299900	-4.500800	-0.687800
H	-2.918500	-4.995800	-1.429200
C	-2.189500	-5.033500	0.595600
H	-2.721000	-5.943600	0.861500
C	-1.381600	-4.376600	1.530000
H	-1.256300	-4.756800	2.540200
C	-0.722200	-3.211100	1.148200
H	-0.082800	-2.680300	1.845600

Optimised cartesian coordinates of **2b**$^{-}$ **(**DFT/UB3LYP/sdd/6-31G(d))

E(Total)= −2461.89169766 a.u.

Ru	0.040889	-0.644015	-0.795643
Cl	-6.816330	0.232314	-1.261490
Cl	-4.542177	-3.463469	2.087499
Cl	-1.817416	-0.099345	4.917572
Cl	2.938096	-2.798299	5.279326
O	0.391101	1.351285	-1.346126
O	1.888918	-1.164642	-1.670276
N	-1.738168	0.349870	-0.034039
N	-0.956643	-1.094631	-2.598737
N	-0.447203	-2.714223	-0.574281
N	1.394537	-0.461402	0.872596
C	-0.466582	2.240444	-0.840173
C	-0.291410	3.650874	-1.012909
C	-1.251541	4.505132	-0.445768
H	-1.114721	5.573152	-0.564419
C	-2.370758	4.046403	0.283409
C	-2.532255	2.662631	0.426325
H	-3.371493	2.266162	0.992435
C	-1.623894	1.747741	-0.143410
C	-3.408316	5.010668	0.914769
C	-4.813374	4.739200	0.300476
H	-5.567735	5.409009	0.742449
H	-5.135691	3.705375	0.473615
H	-4.799225	4.906404	-0.785512
C	-3.063667	6.501223	0.667399
H	-2.094573	6.771845	1.106925
H	-3.831304	7.139067	1.128192
H	-3.031221	6.738098	-0.404229
C	-3.473530	4.788638	2.454290
H	-2.496275	4.985325	2.915175
H	-3.754875	3.758190	2.700231
H	-4.215135	5.461784	2.912261
C	0.933503	4.211325	-1.784907
C	0.922068	5.760714	-1.873398
H	0.034327	6.139947	-2.398467
H	1.808344	6.094295	-2.431765
H	0.960646	6.229239	-0.880765
C	2.248547	3.790059	-1.065819

H	2.279532	4.207678	-0.049713
H	3.121903	4.170079	-1.618634
H	2.326354	2.702229	-0.993307
C	0.946571	3.665984	-3.244173
H	1.021994	2.574995	-3.245482
H	1.808317	4.074655	-3.794539
H	0.030155	3.961859	-3.775876
C	-2.991862	-0.240877	0.113437
C	-4.156347	0.250348	-0.551481
H	-4.081841	1.123254	-1.191424
C	-5.371545	-0.398079	-0.389747
C	-5.535577	-1.540643	0.404991
H	-6.496652	-2.028184	0.519921
C	-4.382378	-2.012779	1.042965
C	-3.139344	-1.402035	0.922188
H	-2.282457	-1.784320	1.464739
C	-1.114629	-0.206765	-3.612574
H	-0.726724	0.788545	-3.411724
C	-1.727351	-0.546344	-4.813150
H	-1.839560	0.206900	-5.589611
C	-2.192831	-1.860488	-4.992944
H	-2.678234	-2.159002	-5.920110
C	-2.017753	-2.781365	-3.961328
H	-2.360107	-3.805083	-4.082349
C	-1.394709	-2.385888	-2.763981
C	-1.132048	-3.280714	-1.629937
C	-1.524735	-4.630517	-1.599460
H	-2.084578	-5.048107	-2.431455
C	-1.200527	-5.430175	-0.505655
H	-1.509664	-6.472744	-0.470883
C	-0.468294	-4.856678	0.546416
H	-0.179391	-5.435673	1.420510
C	-0.114205	-3.514330	0.471888
H	0.446429	-3.036811	1.269444
C	2.705874	-0.304192	0.389781
C	3.764126	0.258684	1.136850
H	3.546117	0.599755	2.144091
C	5.041290	0.410403	0.591680
C	5.247607	-0.042985	-0.734938
H	6.241303	0.061691	-1.160474
C	4.238387	-0.591531	-1.534827
C	2.922320	-0.692342	-0.973103
C	4.508391	-1.058314	-2.988900
C	5.997298	-0.896964	-3.393731
H	6.132092	-1.250983	-4.425799
H	6.664076	-1.486695	-2.749500

H	6.323383	0.151487	-3.358244
C	4.142480	-2.564797	-3.141787
H	3.092208	-2.735319	-2.888557
H	4.764883	-3.182906	-2.478638
H	4.316526	-2.893050	-4.178530
C	3.649860	-0.215606	-3.979024
H	2.586690	-0.312461	-3.742741
H	3.819317	-0.554071	-5.013541
H	3.922307	0.847188	-3.916141
C	6.209378	1.077333	1.361114
C	5.810482	1.489967	2.800364
H	6.670949	1.951950	3.305100
H	5.495069	0.625101	3.398179
H	4.991697	2.220547	2.800522
C	6.669606	2.362379	0.609552
H	5.843149	3.081103	0.533005
H	7.007023	2.133209	-0.409183
H	7.502575	2.846777	1.143462
C	7.409854	0.090368	1.461621
H	7.767570	-0.212563	0.469548
H	7.119428	-0.819155	2.004976
H	8.250824	0.558458	1.996888
C	1.166334	-0.749353	2.208977
C	-0.049132	-0.335385	2.827408
H	-0.760385	0.244544	2.248415
C	-0.296858	-0.661825	4.154360
C	0.593482	-1.399028	4.949150
H	0.377777	-1.636678	5.984259
C	1.775420	-1.809363	4.321373
C	2.081373	-1.514048	3.000556
H	3.005287	-1.873667	2.560115