

Electronic Supplementary Information

Dinuclear $\{[(p\text{-cym})\text{Ru}^{\text{II}}\text{Cl}]_2(\mu\text{-bpytz}^{\bullet-})\}^+$ complex bridged by a radical anion: synthesis, spectroelectrochemical, EPR and theoretical investigation (bpytz = 3,6-bis(3,5-dimethylpyrazolyl)1,2,4,5-tetrazine; *p*-cym = *p*-cymene)

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Fig. S1 Optimised structure of $[1]^+$.

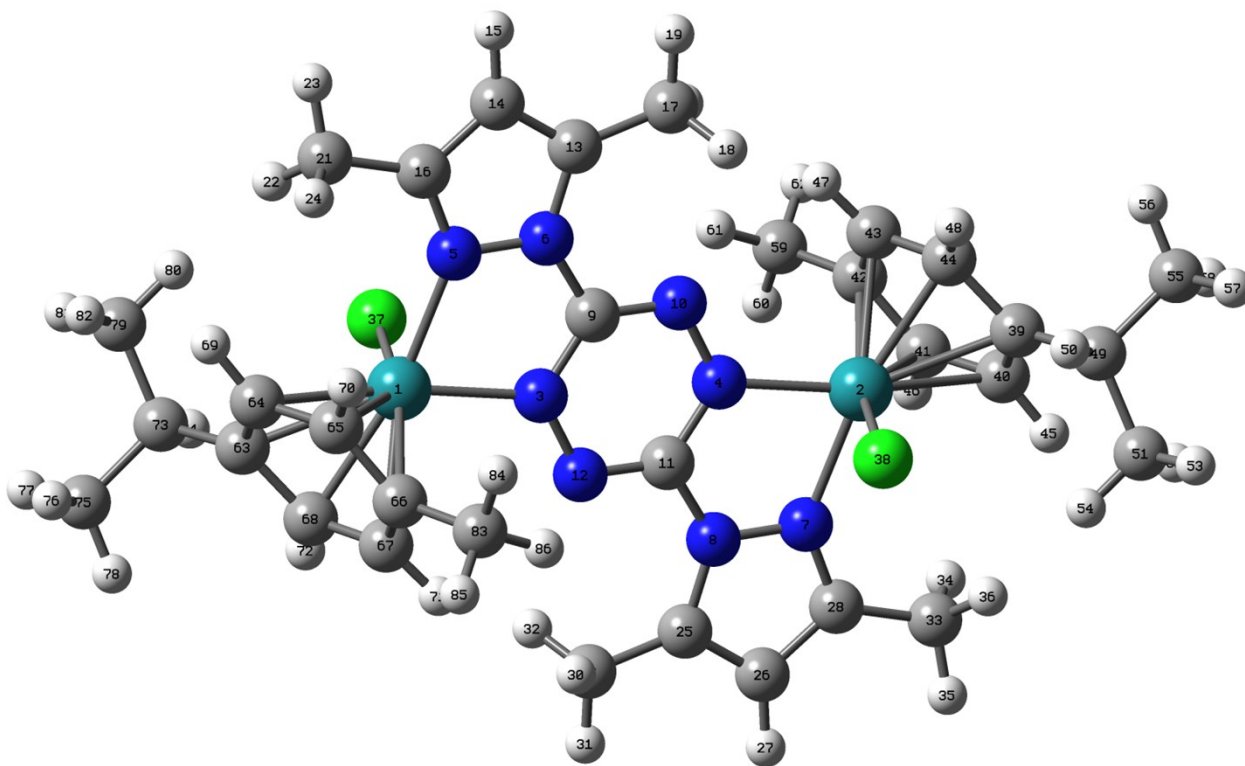


Table S1. Mulliken atomic spin densities for [1]⁺.

Number	Symbol	Value	Number	Symbol	Value	Number	Symbol	Value
1	Ru	0.0185	41	C	-0.0030	81	H	0.0000
2	Ru	0.0185	42	C	0.0133	82	H	0.0000
3	N	0.2976	43	C	-0.0038	83	C	-0.0008
4	N	0.2976	44	C	0.0013	84	H	0.0001
5	N	0.0027	45	H	0.0000	85	H	0.0006
6	N	0.0020	46	H	0.0002	86	H	-0.0001
7	N	0.0027	47	H	0.0000			
8	N	0.0020	48	H	0.0001			
9	C	-0.0845	49	C	0.0001			
10	N	0.2666	50	H	-0.0001			
11	C	-0.0845	51	C	0.0000			
12	N	0.2666	52	H	0.0000			
13	C	-0.0054	53	H	0.0000			
14	C	-0.0020	54	H	0.0000			
15	H	0.0002	55	C	-0.0001			
16	C	-0.0084	56	H	0.0000			
17	C	0.0007	57	H	-0.0001			
18	H	0.0000	58	H	0.0000			
19	H	-0.0002	59	C	-0.0008			
20	H	-0.0002	60	H	0.0001			
21	C	0.0008	61	H	-0.0001			
22	H	-0.0004	62	H	0.0006			
23	H	0.0000	63	C	-0.0026			
24	H	-0.0005	64	C	0.0012			
25	C	-0.0054	65	C	-0.0030			
26	C	-0.0020	66	C	0.0133			
27	H	0.0002	67	C	-0.0038			
28	C	-0.0084	68	C	0.0013			
29	C	0.0007	69	H	0.0000			
30	H	-0.0002	70	H	0.0002			
31	H	-0.0002	71	H	0.0000			
32	H	0.0000	72	H	0.0001			
33	C	0.0008	73	C	0.0001			
34	H	-0.0005	74	H	-0.0001			
35	H	0.0000	75	C	-0.0001			
36	H	-0.0004	76	H	0.0000			
37	Cl	0.0063	77	H	-0.0001			
38	Cl	0.0063	78	H	0.0000			
39	C	-0.0026	79	C	0.0000			
40	C	0.0012	80	H	0.0000			

Table S2. Calculated energies of Kohn-Sham molecular orbitals (MO) at the B3LYP Level and the contributions of various molecular groups to the MOs of [1]⁺.

α spin orbitals							β spin orbitals						
Sr. No.	MO's	Energy(eV)	Contribution of the group to MO (%)				Sr. No.	MO's	Energy(eV)	Contribution of the group to MO (%)			
			bpytz	Cl	Ru	p-cym				bpytz	Cl	Ru	p-cym
189	LUMO+10	-1.79	77	0	20	3							
188	LUMO+9	-2.85	27	2	14	57	188	LUMO+10	-2.79	44	1	13	42
187	LUMO+8	-2.89	3	1	21	75	187	LUMO+9	-2.86	4	1	22	74
186	LUMO+7	-2.93	6	0	24	69	186	LUMO+8	-2.9	8	0	25	67
185	LUMO+6	-2.98	4	1	20	75	185	LUMO+7	-2.97	4	1	21	74
184	LUMO+5	-3.21	68	0	7	25	184	LUMO+6	-3.11	49	1	10	40
183	LUMO+4	-3.73	16	0	53	32	183	LUMO+5	-3.66	22	0	48	30
182	LUMO+3	-3.75	16	0	51	32	182	LUMO+4	-3.71	17	0	49	34
181	LUMO+2	-4.01	17	13	47	23	181	LUMO+3	-3.98	25	11	44	20
180	LUMO+1	-4.05	6	16	50	28	180	LUMO+2	-4.03	6	16	50	29
179	LUMO	-4.23	84	3	6	7	179	LUMO+1	-4.15	76	4	10	9
178	HOMO	-7.21	77	2	15	5	178	LUMO	-4.85	83	2	8	7
177	HOMO-1	-8.14	6	42	39	13	177	HOMO	-8.11	7	38	41	14
176	HOMO-2	-8.18	6	44	38	12	176	HOMO-1	-8.17	5	44	38	13
175	HOMO-3	-8.33	11	35	46	8	175	HOMO-2	-8.26	13	31	47	9
174	HOMO-4	-8.51	13	58	25	4	174	HOMO-3	-8.41	9	48	37	6
173	HOMO-5	-8.89	15	49	23	12	173	HOMO-4	-8.85	20	52	18	10
172	HOMO-6	-8.96	23	33	30	13	172	HOMO-5	-8.93	18	38	30	13
171	HOMO-7	-9.26	69	20	9	1	171	HOMO-6	-9.09	77	13	7	2
170	HOMO-8	-9.37	32	14	50	5	170	HOMO-7	-9.35	34	18	44	5
169	HOMO-9	-9.41	39	8	48	5	169	HOMO-8	-9.36	33	16	46	5

168	HOMO-10	-9.68	33	32	27	8		168	HOMO-9	-9.58	31	31	31	7
167	HOMO-11	-9.9	21	31	39	10		167	HOMO-10	-9.8	18	33	41	8
166	HOMO-12	-10.07	70	11	13	6								
165	HOMO-13	-10.12	63	1	16	20								

Table S3. Various bond lengths (Å) in optimised [1]⁺.

Definition*	Value	Definition*	Value	Definition*	Value
R (1,3)	2.0669	R (21,22)	1.0941	R (63,73)	1.5170
R (1,5)	2.1108	R (21,23)	1.0927	R (64,65)	1.4353
R (1,37)	2.4326	R (21,24)	1.0963	R (64,69)	1.0823
R (1,63)	2.3494	R (25,26)	1.3777	R (65,66)	1.4136
R (1,64)	2.3233	R (25,29)	1.4926	R (65,70)	1.0857
R (1,65)	2.2645	R (26,27)	1.0803	R (66,67)	1.4348
R (1,66)	2.3045	R (26,28)	1.4138	R (66,83)	1.5046
R (1,67)	2.2405	R (28,33)	1.4947	R (67,68)	1.4078
R (1,68)	2.2537	R (29,30)	1.0947	R (67,71)	1.0844
R (2,4)	2.0669	R (29,31)	1.0929	R (68,72)	1.0840
R (2,7)	2.1108	R (29,32)	1.0937	R (73,74)	1.0967
R (2,38)	2.4326	R (33,34)	1.0963	R (73,75)	1.5460
R (2,39)	2.3494	R (33,35)	1.0927	R (73,79)	1.5331
R (2,40)	2.3233	R (33,36)	1.0941	R (75,76)	1.0963
R (2,41)	2.2645	R (39,40)	1.4060	R (75,77)	1.0949
R (2,42)	2.3045	R (39,44)	1.4410	R (75,78)	1.0957
R (2,43)	2.2405	R (39,49)	1.5170	R (79,80)	1.0945
R (2,44)	2.2537	R (40,41)	1.4353	R (79,81)	1.0945
R (3,9)	1.3465	R (40,45)	1.0823	R (79,82)	1.0971
R (3,12)	1.3690	R (41,42)	1.4136	R (83,84)	1.0937
R (4,10)	1.3690	R (41,46)	1.0857	R (83,85)	1.0974
R (4,11)	1.3465	R (42,43)	1.4348	R (83,86)	1.0943
R (5,6)	1.3749	R (42,59)	1.5046		
R (5,16)	1.3324	R (43,44)	1.4078		
R (6,9)	1.3981	R (43,47)	1.0844		
R (6,13)	1.3778	R (44,48)	1.0840		
R (7,8)	1.3749	R (49,50)	1.0967		
R (7,28)	1.3324	R (49,51)	1.5331		
R (8,11)	1.3981	R (49,55)	1.5460		
R (8,25)	1.3778	R (51,52)	1.0971		
R (9,10)	1.3166	R (51,53)	1.0945		
R (11,12)	1.3166	R (51,54)	1.0945		
R (13,14)	1.3777	R (55,56)	1.0957		
R (13,17)	1.4926	R (55,57)	1.0949		
R (14,15)	1.0803	R (55,58)	1.0963		
R (14,16)	1.4138	R (59,60)	1.0937		
R (16,21)	1.4947	R (59,61)	1.0943		
R (17,18)	1.0937	R (59,62)	1.0974		
R (17,19)	1.0929	R (63,64)	1.4060		
R (17,20)	1.0947	R (63,68)	1.4410		

* For the atomic indices refer to Figure S1

Table S4 Various bond angles (°) in optimised [1]⁺.

Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value
A(3,1,5)	75.74	A(7,2,40)	105.45	A(6,9,10)	119.01	A(30,29,32)	107.50	A(49,51,54)	110.98	A(63,73,74)	106.11
A(3,1,37)	84.31	A(7,2,41)	98.31	A(4,10,9)	114.85	A(31,29,32)	109.10	A(52,51,53)	106.99	A(63,73,75)	108.79
A(3,1,63)	151.34	A(7,2,42)	116.18	A(4,11,8)	113.96	A(28,33,34)	111.50	A(52,51,54)	109.38	A(63,73,79)	114.47
A(3,1,64)	163.31	A(7,2,43)	150.43	A(4,11,12)	127.03	A(28,33,35)	110.00	A(53,51,54)	107.71	A(74,73,75)	108.33
A(3,1,65)	127.02	A(7,2,44)	168.04	A(8,11,12)	119.01	A(28,33,36)	110.80	A(49,55,56)	112.00	A(74,73,79)	107.46
A(3,1,66)	99.07	A(38,2,39)	89.87	A(3,12,11)	114.85	A(34,33,35)	107.70	A(49,55,57)	109.74	A(75,73,79)	111.37
A(3,1,67)	94.57	A(38,2,40)	112.37	A(6,13,14)	105.55	A(34,33,36)	108.30	A(49,55,58)	111.12	A(73,75,76)	111.12
A(3,1,68)	115.97	A(38,2,41)	148.36	A(6,13,17)	125.26	A(35,33,36)	108.40	A(56,55,57)	107.86	A(73,75,77)	109.74
A(5,1,37)	84.24	A(38,2,42)	159.54	A(14,13,17)	129.19	A(2,39,49)	130.50	A(56,55,58)	108.01	A(73,75,78)	112.00
A(5,1,63)	131.64	A(38,2,43)	123.12	A(13,14,15)	126.07	A(40,39,44)	117.20	A(57,55,58)	107.97	A(76,75,77)	107.97
A(5,1,64)	105.45	A(38,2,44)	94.25	A(13,14,16)	107.45	A(40,39,49)	123.80	A(42,59,60)	111.41	A(76,75,78)	108.01
A(5,1,65)	98.31	A(39,2,41)	64.81	A(15,14,16)	126.48	A(44,39,49)	118.90	A(42,59,61)	111.26	A(77,75,78)	107.86
A(5,1,66)	116.18	A(39,2,42)	77.46	A(5,16,14)	109.34	A(2,40,45)	127.20	A(42,59,62)	110.13	A(73,79,80)	110.98
A(5,1,67)	150.43	A(39,2,43)	65.43	A(5,16,21)	122.95	A(39,40,41)	121.10	A(60,59,61)	108.37	A(73,79,81)	109.40
A(5,1,68)	168.04	A(40,2,42)	65.17	A(14,16,21)	127.71	A(39,40,45)	119.90	A(60,59,62)	107.79	A(73,79,82)	112.21
A(37,1,63)	89.87	A(40,2,43)	76.17	A(13,17,18)	111.68	A(41,40,45)	118.90	A(61,59,62)	107.74	A(80,79,81)	107.71
A(37,1,64)	112.37	A(40,2,44)	64.13	A(13,17,19)	108.72	A(2,41,46)	125.30	A(1,63,73)	130.54	A(80,79,82)	109.38
A(37,1,65)	148.36	A(41,2,43)	65.00	A(13,17,20)	111.20	A(40,41,42)	122.10	A(64,63,68)	117.24	A(81,79,82)	106.99
A(37,1,66)	159.54	A(41,2,44)	76.80	A(18,17,19)	109.12	A(40,41,46)	118.90	A(64,63,73)	123.83	A(66,83,84)	111.41
A(37,1,67)	123.12	A(42,2,44)	66.04	A(18,17,20)	107.48	A(42,41,46)	119.00	A(68,63,73)	118.92	A(66,83,85)	110.13
A(37,1,68)	94.25	A(1,3,9)	118.35	A(19,17,20)	108.57	A(2,42,59)	129.30	A(1,64,69)	127.20	A(66,83,86)	111.26
A(63,1,65)	64.81	A(1,3,12)	122.90	A(16,21,22)	110.84	A(41,42,43)	116.40	A(63,64,65)	121.06	A(84,83,85)	107.79
A(63,1,66)	77.46	A(9,3,12)	118.13	A(16,21,23)	109.96	A(41,42,59)	122.40	A(63,64,69)	119.94	A(84,83,86)	108.37
A(63,1,67)	65.43	A(2,4,10)	122.90	A(16,21,24)	111.54	A(43,42,59)	121.20	A(65,64,69)	118.92	A(85,83,86)	107.74
A(64,1,66)	65.17	A(2,4,11)	118.35	A(22,21,23)	108.36	A(2,43,47)	122.20	A(1,65,70)	125.34		<i>Cont...</i>
A(64,1,67)	76.17	A(10,4,11)	118.13	A(22,21,24)	108.32	A(42,43,44)	121.80	A(64,65,66)	122.06		

A(64,1,68)	64.13	A(1,5,6)	114.36	A(23,21,24)	107.70	A(42,43,47)	118.90	A(64,65,70)	118.95		
A(65,1,67)	65.00	A(1,5,16)	138.70	A(8,25,26)	105.55	A(44,43,47)	119.10	A(66,65,70)	118.99		
A(65,1,68)	76.80	A(6,5,16)	106.62	A(8,25,29)	125.26	A(2,44,48)	123.50	A(1,66,83)	129.29		
A(66,1,68)	66.04	A(5,6,9)	116.75	A(26,25,29)	129.19	A(39,44,43)	121.20	A(65,66,67)	116.37		
A(4,2,7)	75.74	A(5,6,13)	111.03	A(25,26,27)	126.07	A(39,44,48)	119.10	A(65,66,83)	122.40		
A(4,2,38)	84.31	A(9,6,13)	132.20	A(25,26,28)	107.45	A(43,44,48)	119.60	A(67,66,83)	121.21		
A(4,2,39)	151.34	A(2,7,8)	114.36	A(27,26,28)	126.48	A(39,49,50)	106.10	A(1,67,71)	122.23		
A(4,2,40)	163.31	A(2,7,28)	138.70	A(7,28,26)	109.34	A(39,49,51)	114.50	A(66,67,68)	121.83		
A(4,2,41)	127.02	A(8,7,28)	106.62	A(7,28,33)	122.95	A(39,49,55)	108.80	A(66,67,71)	118.92		
A(4,2,42)	99.07	A(7,8,11)	116.75	A(26,28,33)	127.71	A(50,49,51)	107.50	A(68,67,71)	119.06		
A(4,2,43)	94.57	A(7,8,25)	111.03	A(25,29,30)	111.20	A(50,49,55)	108.30	A(1,68,72)	123.52		
A(4,2,44)	115.97	A(11,8,25)	132.20	A(25,29,31)	108.72	A(51,49,55)	111.40	A(63,68,67)	121.24		
A(7,2,38)	84.24	A(3,9,6)	113.96	A(25,29,32)	111.68	A(49,51,52)	112.20	A(63,68,72)	119.12		
A(7,2,39)	131.64	A(3,9,10)	127.03	A(30,29,31)	108.57	A(49,51,53)	109.40	A(67,68,72)	119.59		

* For the atomic indices refer to Figure S1

Table S5. Various dihedral angles (°) in optimised [1]⁺.

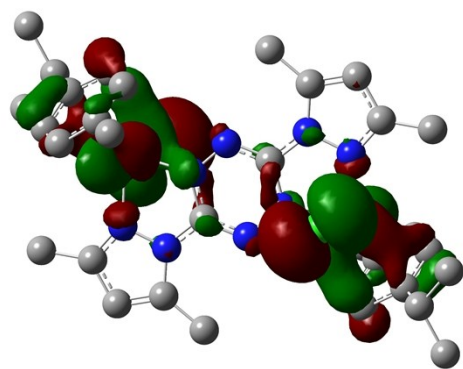
Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value
D(5,1,3,9)	-8.5	D(37,1,64,69)	-61.7	D(43,2,4,10)	-29.1	D(44,39,49,55)	-79.4	D(50,49,55,58)	179.7	D(67,66,83,85)	-82.8
D(5,1,3,12)	-179.0	D(66,1,64,69)	140.5	D(43,2,4,11)	160.2	D(39,40,41,42)	3.5	D(51,49,55,56)	-177.4	D(67,66,83,86)	36.6
D(37,1,3,9)	77.0	D(67,1,64,69)	177.9	D(44,2,4,10)	1.8	D(39,40,41,46)	-177.0	D(51,49,55,57)	-57.6	D(66,67,68,63)	-1.4
D(37,1,3,12)	-93.8	D(68,1,64,69)	-145.3	D(44,2,4,11)	-168.9	D(45,40,41,42)	-180.0	D(51,49,55,58)	61.7	D(66,67,68,72)	176.0
D(63,1,3,9)	156.2	D(3,1,65,70)	68.7	D(4,2,7,8)	-6.1	D(45,40,41,46)	0.1	D(68,63,64,65)	-0.7	D(71,67,68,63)	-176.4
D(63,1,3,12)	-14.6	D(5,1,65,70)	-9.7	D(4,2,7,28)	-178.5	D(40,41,42,43)	-5.0	D(68,63,64,69)	176.0	D(71,67,68,72)	1.0
D(64,1,3,9)	-105.0	D(37,1,65,70)	-102.2	D(38,2,7,8)	79.5	D(40,41,42,59)	176.8	D(73,63,64,65)	-179.8	D(63,73,75,76)	65.4
D(64,1,3,12)	84.5	D(63,1,65,70)	-142.0	D(38,2,7,28)	-92.9	D(46,41,42,43)	175.1	D(73,63,64,69)	-3.1	D(63,73,75,77)	-175.3
D(65,1,3,9)	-98.2	D(67,1,65,70)	144.7	D(39,2,7,8)	164.1	D(46,41,42,59)	-3.1	D(64,63,68,67)	3.1	D(63,73,75,78)	-55.5
D(65,1,3,12)	91.0	D(68,1,65,70)	-178.6	D(39,2,7,28)	-8.2	D(41,42,43,44)	2.6	D(64,63,68,72)	-174.3	D(74,73,75,76)	-179.7
D(66,1,3,9)	-123.0	D(3,1,66,83)	28.4	D(40,2,7,8)	-168.9	D(41,42,43,47)	-172.0	D(73,63,68,67)	-177.8	D(74,73,75,77)	-60.4
D(66,1,3,12)	65.9	D(5,1,66,83)	-50.1	D(40,2,7,28)	18.7	D(59,42,43,44)	-179.0	D(73,63,68,72)	4.8	D(74,73,75,78)	59.4
D(67,1,3,9)	-160.0	D(37,1,66,83)	126.5	D(41,2,7,8)	-132.3	D(59,42,43,47)	5.8	D(1,63,73,74)	48.1	D(79,73,75,76)	-61.7
D(67,1,3,12)	29.1	D(63,1,66,83)	179.5	D(41,2,7,28)	55.3	D(2,42,59,60)	-70.0	D(1,63,73,75)	164.5	D(79,73,75,77)	57.6
D(68,1,3,9)	168.9	D(64,1,66,83)	-145.8	D(42,2,7,8)	-99.4	D(2,42,59,61)	51.1	D(1,63,73,79)	-70.2	D(79,73,75,78)	177.4
D(68,1,3,12)	-1.8	D(68,1,66,83)	142.9	D(42,2,7,28)	88.3	D(2,42,59,62)	170.4	D(64,63,73,74)	142.2	D(63,73,79,80)	57.3
D(3,1,5,6)	6.1	D(3,1,67,71)	-15.4	D(43,2,7,8)	-79.8	D(41,42,59,60)	20.4	D(64,63,73,75)	-101.5	D(63,73,79,81)	176.0
D(3,1,5,16)	178.5	D(5,1,67,71)	-84.4	D(43,2,7,28)	107.8	D(41,42,59,61)	141.5	D(64,63,73,79)	23.8	D(63,73,79,82)	-65.4
D(37,1,5,6)	-79.5	D(37,1,67,71)	70.8	D(44,2,7,8)	162.8	D(41,42,59,62)	-99.2	D(68,63,73,74)	-36.9	D(74,73,79,80)	-60.3
D(37,1,5,16)	92.9	D(63,1,67,71)	143.2	D(44,2,7,28)	-9.6	D(43,42,59,60)	-158.0	D(68,63,73,75)	79.4	D(74,73,79,81)	58.4
D(63,1,5,6)	-164.0	D(64,1,67,71)	178.7	D(4,2,39,49)	90.5	D(43,42,59,61)	-36.6	D(68,63,73,79)	-155.3	D(74,73,79,82)	177.0
D(63,1,5,16)	8.2	D(65,1,67,71)	-144.4	D(7,2,39,49)	-69.5	D(43,42,59,62)	82.8	D(63,64,65,66)	-3.5	D(75,73,79,80)	-178.8
D(64,1,5,6)	168.9	D(3,1,68,72)	-54.2	D(38,2,39,49)	12.7	D(42,43,44,39)	1.4	D(63,64,65,70)	176.6	D(75,73,79,81)	-60.1
D(64,1,5,16)	-18.7	D(5,1,68,72)	113.8	D(41,2,39,49)	-147.7	D(42,43,44,48)	-176.0	D(69,64,65,66)	179.8	D(75,73,79,82)	58.5
D(65,1,5,6)	132.3	D(37,1,68,72)	31.5	D(42,2,39,49)	176.5	D(47,43,44,39)	176.4	D(69,64,65,70)	-0.1	D(27,26,28,7)	179.4
D(65,1,5,16)	-55.3	D(64,1,68,72)	144.4	D(43,2,39,49)	139.7	D(47,43,44,48)	-1.0	D(64,65,66,67)	5.0	D(27,26,28,33)	-1.0

D(66,1,5,6)	99.4	D(65,1,68,72)	-179.2	D(4,2,40,45)	-120.2	D(39,49,51,52)	65.4	D(64,65,66,83)	-176.8	D(7,28,33,34)	-69.5
D(66,1,5,16)	-88.3	D(66,1,68,72)	-142.8	D(7,2,40,45)	-28.4	D(39,49,51,53)	-176.0	D(70,65,66,67)	-175.1	D(7,28,33,35)	171.1
D(67,1,5,6)	79.8	D(7,2,4,10)	179.3	D(38,2,40,45)	61.7	D(39,49,51,54)	-57.3	D(70,65,66,83)	3.1	D(7,28,33,36)	51.3
D(67,1,5,16)	-108.0	D(7,2,4,11)	8.5	D(42,2,40,45)	-140.5	D(50,49,51,52)	-177.0	D(65,66,67,68)	-2.6	D(26,28,33,34)	111.0
D(68,1,5,6)	-163.0	D(38,2,4,10)	93.8	D(43,2,40,45)	-177.9	D(50,49,51,53)	-58.4	D(65,66,67,71)	172.4	D(26,28,33,35)	-8.4
D(68,1,5,16)	9.6	D(38,2,4,11)	-77.0	D(44,2,40,45)	145.3	D(50,49,51,54)	60.3	D(83,66,67,68)	179.2	D(26,28,33,36)	-128.2
D(3,1,63,73)	-90.5	D(39,2,4,10)	14.6	D(4,2,41,46)	-68.7	D(55,49,51,52)	-58.5	D(83,66,67,71)	-5.8	D(44,39,40,41)	0.7
D(5,1,63,73)	69.5	D(39,2,4,11)	-156.2	D(7,2,41,46)	9.7	D(55,49,51,53)	60.1	D(1,66,83,84)	70.0	D(44,39,40,45)	-176.0
D(37,1,63,73)	-12.7	D(40,2,4,10)	-84.5	D(38,2,41,46)	102.2	D(55,49,51,54)	178.8	D(1,66,83,85)	-170.4	D(49,39,40,41)	179.8
D(65,1,63,73)	147.7	D(40,2,4,11)	104.8	D(39,2,41,46)	142.0	D(39,49,55,56)	55.5	D(1,66,83,86)	-51.1	D(49,39,40,45)	3.1
D(66,1,63,73)	-177.0	D(41,2,4,10)	-91.0	D(43,2,41,46)	-144.7	D(39,49,55,57)	175.3	D(65,66,83,84)	-20.4	D(40,39,44,43)	-3.1
D(67,1,63,73)	-140.0	D(41,2,4,11)	98.2	D(44,2,41,46)	178.6	D(39,49,55,58)	-65.4	D(65,66,83,85)	99.2	D(40,39,44,48)	174.3
D(3,1,64,69)	120.2	D(42,2,4,10)	-65.9	D(4,2,42,59)	-28.4	D(50,49,55,56)	-59.4	D(65,66,83,86)	-141.5	D(49,39,44,43)	177.8
D(5,1,64,69)	28.4	D(42,2,4,11)	123.4	D(7,2,42,59)	50.1	D(50,49,55,57)	60.4	D(67,66,83,84)	157.7	D(49,39,44,48)	-4.8
D(1,3,9,6)	9.3	D(1,3,12,11)	170.9	D(12,3,9,10)	-0.2	D(17,13,14,15)	0.0	D(10,4,11,8)	179.5	D(2,39,49,50)	-48.1
D(38,2,42,59)	-127.0	D(5,6,13,14)	-0.3	D(5,16,21,24)	69.5	D(17,13,14,16)	-180.0	D(10,4,11,12)	0.2	D(2,39,49,51)	70.2
D(39,2,42,59)	-179.0	D(5,6,13,17)	179.5	D(14,16,21,22)	128.2	D(6,13,17,18)	-54.8	D(1,5,6,9)	-3.4	D(2,39,49,55)	-164.5
D(40,2,42,59)	145.8	D(9,6,13,14)	178.3	D(14,16,21,23)	8.4	D(6,13,17,19)	-175.2	D(1,5,6,13)	175.4	D(40,39,49,50)	-142.1
D(44,2,42,59)	-143.0	D(9,6,13,17)	-1.8	D(14,16,21,24)	-111.0	D(6,13,17,20)	65.3	D(16,5,6,9)	-178.0	D(40,39,49,51)	-23.8
D(4,2,43,47)	15.4	D(2,7,8,11)	3.4	D(8,25,26,27)	-179.8	D(14,13,17,18)	125.1	D(16,5,6,13)	0.7	D(40,39,49,55)	101.5
D(7,2,43,47)	84.4	D(2,7,8,25)	-175.4	D(8,25,26,28)	0.1	D(14,13,17,19)	4.6	D(1,5,16,14)	-174.0	D(44,39,49,50)	36.9
D(38,2,43,47)	-70.8	D(28,7,8,11)	178.2	D(29,25,26,27)	0.0	D(14,13,17,20)	-114.9	D(1,5,16,21)	6.1	D(44,39,49,51)	155.3
D(39,2,43,47)	-143.0	D(28,7,8,25)	-0.7	D(29,25,26,28)	180.0	D(13,14,16,5)	0.6	D(6,5,16,14)	-0.8	D(7,8,25,26)	0.3
D(40,2,43,47)	-179.0	D(2,7,28,26)	173.5	D(8,25,29,30)	-65.3	D(13,14,16,21)	-179.0	D(6,5,16,21)	178.8	D(7,8,25,29)	-179.5
D(41,2,43,47)	144.4	D(2,7,28,33)	-6.1	D(8,25,29,31)	175.2	D(15,14,16,5)	-179.4	D(5,6,9,3)	-3.6	D(11,8,25,26)	-178.3
D(4,2,44,48)	54.2	D(8,7,28,26)	0.8	D(8,25,29,32)	54.8	D(15,14,16,21)	1.0	D(5,6,9,10)	177.0	D(11,8,25,29)	1.8
D(7,2,44,48)	-114.0	D(8,7,28,33)	-178.8	D(26,25,29,30)	114.9	D(5,16,21,22)	-51.3	D(13,6,9,3)	177.8	D(3,9,10,4)	0.1
D(38,2,44,48)	-31.5	D(7,8,11,4)	3.6	D(26,25,29,31)	-4.6	D(5,16,21,23)	-171.1	D(13,6,9,10)	-1.6	D(6,9,10,4)	179.5
D(40,2,44,48)	-144.0	D(7,8,11,12)	-177.0	D(12,3,9,6)	-179.0	D(11,4,10,9)	-0.1	D(8,11,12,3)	-179.5	D(4,11,12,3)	-0.1

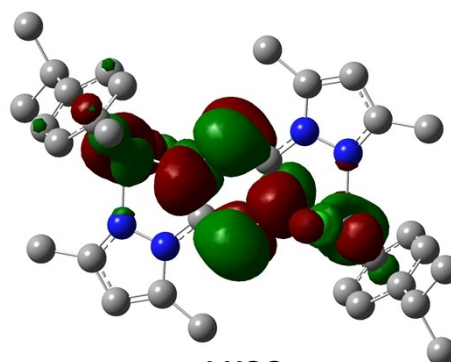
D(41,2,44,48)	179.2	D(25,8,11,4)	-177.8	D(25,26,28,7)	-0.6	D(2,4,11,8)	-9.3	D(6,13,14,15)	179.8	D(9,3,12,11)	0.1
D(42,2,44,48)	142.8	D(25,8,11,12)	1.6	D(1,3,9,10)	-171.0	D(2,4,11,12)	171.3	D(6,13,14,16)	-0.1	D(2,4,10,9)	-171.0

* For the atomic indices refer to Figure S1

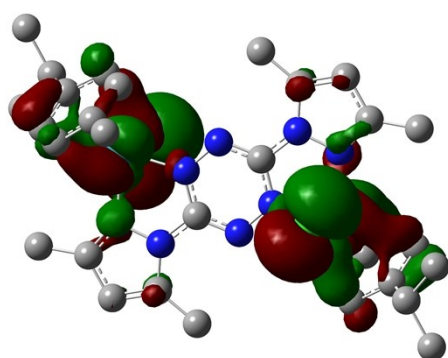
Fig. S2 Pictorial representations of important Kohn-Sham molecular orbitals of $[1]^{2+}$.



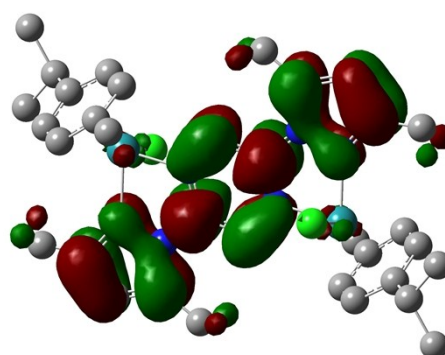
HOSO



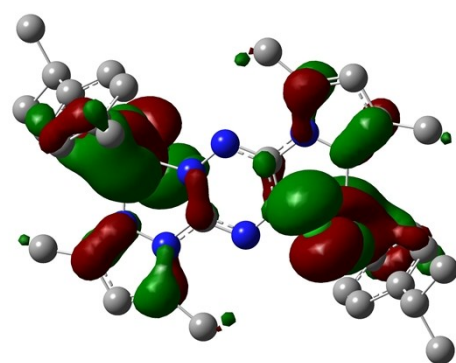
LUSO



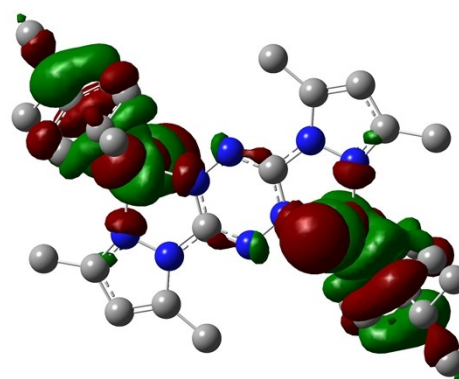
HOSO - 1



LUSO + 1



HOSO - 2



LUSO + 2

Table S6. Calculated energies of Kohn-Sham molecular orbitals (MO) at the B3LYP Level and the contributions of various molecular groups to the MOs of [1]²⁺.

Sr. No.	MO's	Energy(eV)	Contribution of the group to MO (%)			
			bpytz	Cl	Ru	p-cym
188	LUMO+10	-5.73	15	2	14	70
187	LUMO+9	-5.76	2	2	16	82
186	LUMO+8	-5.84	6	0	20	74
185	LUMO+7	-5.88	3	0	16	80
184	LUMO+6	-6.17	79	0	4	16
183	LUMO+5	-6.72	17	0	53	30
182	LUMO+4	-6.72	17	0	55	29
181	LUMO+3	-7.19	6	17	52	26
180	LUMO+2	-7.19	6	18	50	26
179	LUMO+1	-7.71	97	0	2	2
178	LUMO	-9.04	77	2	16	4
177	HOMO	-11.13	5	42	42	10
176	HOMO-1	-11.17	5	46	38	10
175	HOMO-2	-11.21	14	28	48	10
174	HOMO-3	-11.49	15	54	28	4
173	HOMO-4	-11.86	14	58	16	12
172	HOMO-5	-11.92	25	40	22	14
171	HOMO-6	-12.16	79	16	4	0
170	HOMO-7	-12.38	34	10	48	6
169	HOMO-8	-12.44	37	10	48	6
168	HOMO-9	-12.75	20	32	40	8
167	HOMO-10	-12.94	32	16	38	12

Table S7 Various bond lengths (Å) in optimised [1]²⁺

Definition*	Value	Definition*	Value	Definition*	Value
R (1,3)	2.0310	R(21,22)	1.0943	R(63,73)	1.5140
R (1,5)	2.1000	R(21,23)	1.0921	R(64,65)	1.4337
R (1,37)	2.4190	R(21,24)	1.0959	R(64,69)	1.0823
R (1,63)	2.3990	R(25,26)	1.3716	R(65,66)	1.4116
R (1,64)	2.3450	R(25,29)	1.4916	R(65,70)	1.0857
R (1,65)	2.3010	R(26,27)	1.0805	R(66,67)	1.4349
R (1,66)	2.3530	R(26,28)	1.4201	R(66,83)	1.5036
R (1,67)	2.2700	R(28,33)	1.4931	R(67,68)	1.4073
R (1,68)	2.2800	R(29,30)	1.0952	R(67,71)	1.0849
R (2,4)	2.0310	R(29,31)	1.0922	R(68,72)	1.0843
R (2,7)	2.1000	R(29,32)	1.0946	R(73,74)	1.0967
R (2,38)	2.4190	R(33,34)	1.0959	R(73,75)	1.5498
R (2,39)	2.3990	R(33,35)	1.0921	R(73,79)	1.5332
R (2,40)	2.3450	R(33,36)	1.0943	R(75,76)	1.0957
R (2,41)	2.3010	R(39,40)	1.4068	R(75,77)	1.0942
R (2,42)	2.3530	R(39,44)	1.4403	R(75,78)	1.0954
R (2,43)	2.2700	R(39,49)	1.5140	R(79,80)	1.0949
R (2,44)	2.2800	R(40,41)	1.4337	R(79,81)	1.0938
R (3,9)	1.3670	R(40,45)	1.0823	R(79,82)	1.0966
R (3,12)	1.3210	R(41,42)	1.4116	R(83,84)	1.0933
R (4,10)	1.3210	R(41,46)	1.0857	R(83,85)	1.0976
R (4,11)	1.3670	R(42,43)	1.4349	R(83,86)	1.0942
R (5,6)	1.3840	R(42,59)	1.5036		
R (5,16)	1.3300	R(43,44)	1.4073		
R (6,9)	1.3770	R(43,47)	1.0849		
R (6,13)	1.3900	R(44,48)	1.0843		
R (7,8)	1.3840	R(49,50)	1.0967		
R (7,28)	1.3300	R(49,51)	1.5332		
R (8,11)	1.3770	R(49,55)	1.5498		
R (8,25)	1.3900	R(51,52)	1.0966		
R (9,10)	1.3260	R(51,53)	1.0938		
R (11,12)	1.3260	R(51,54)	1.0949		
R (13,14)	1.3720	R(55,56)	1.0954		
R (13,17)	1.4920	R(55,57)	1.0942		
R (14,15)	1.0810	R(55,58)	1.0957		
R (14,16)	1.4200	R(59,60)	1.0933		
R (16,21)	1.4930	R(59,61)	1.0942		
R (17,18)	1.0950	R(59,62)	1.0976		
R (17,19)	1.0920	R(63,64)	1.4068		
R (17,20)	1.0950	R(63,68)	1.4403		

Table S8 Various bond angles (°) in optimised [1]²⁺.

Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value
A(3,1,5)	77.03	A(7,2,40)	104.71	A(6,9,10)	120.44	A(30,29,32)	108.01	A(49,51,54)	111.36	A(63,73,74)	106.40
A(3,1,37)	83.67	A(7,2,41)	99.18	A(4,10,9)	117.72	A(31,29,32)	108.68	A(52,51,53)	106.88	A(63,73,75)	108.06
A(3,1,63)	150.60	A(7,2,42)	118.15	A(4,11,8)	115.21	A(28,33,34)	111.37	A(52,51,54)	109.42	A(63,73,79)	114.64
A(3,1,64)	166.40	A(7,2,43)	152.36	A(4,11,12)	124.34	A(28,33,35)	110.00	A(53,51,54)	107.52	A(74,73,75)	108.13
A(3,1,65)	130.60	A(7,2,44)	165.81	A(8,11,12)	120.44	A(28,33,36)	110.79	A(49,55,56)	112.23	A(74,73,79)	107.96
A(3,1,66)	103.10	A(38,2,39)	88.03	A(3,12,11)	117.72	A(34,33,35)	107.69	A(49,55,57)	109.22	A(75,73,79)	111.35
A(3,1,67)	97.11	A(38,2,40)	109.93	A(6,13,14)	105.23	A(34,33,36)	108.60	A(49,55,58)	111.20	A(73,75,76)	111.20
A(3,1,68)	116.50	A(38,2,41)	145.59	A(6,13,17)	125.09	A(35,33,36)	108.28	A(56,55,57)	107.81	A(73,75,77)	109.22
A(5,1,37)	84.05	A(38,2,42)	157.63	A(14,13,17)	129.68	A(2,39,49)	131.48	A(56,55,58)	108.23	A(73,75,78)	112.23
A(5,1,63)	130.10	A(38,2,43)	122.56	A(13,14,15)	126.00	A(40,39,44)	116.80	A(57,55,58)	108.00	A(76,75,77)	108.00
A(5,1,64)	104.70	A(38,2,44)	92.98	A(13,14,16)	107.94	A(40,39,49)	123.88	A(42,59,60)	111.67	A(76,75,78)	108.23
A(5,1,65)	99.18	A(39,2,41)	63.59	A(15,14,16)	126.06	A(44,39,49)	119.31	A(42,59,61)	111.72	A(77,75,78)	107.81
A(5,1,66)	118.20	A(39,2,42)	75.62	A(5,16,14)	109.41	A(2,40,45)	127.00	A(42,59,62)	109.51	A(73,79,80)	111.36
A(5,1,67)	152.40	A(39,2,43)	64.16	A(5,16,21)	123.30	A(39,40,41)	121.43	A(60,59,61)	108.70	A(73,79,81)	109.23
A(5,1,68)	165.80	A(40,2,42)	63.94	A(14,16,21)	127.29	A(39,40,45)	119.75	A(60,59,62)	107.65	A(73,79,82)	112.22
A(37,1,63)	88.03	A(40,2,43)	74.97	A(13,17,18)	111.79	A(41,40,45)	118.81	A(61,59,62)	107.42	A(80,79,81)	107.52
A(37,1,64)	109.90	A(40,2,44)	63.23	A(13,17,19)	108.64	A(2,41,46)	125.51	A(1,63,73)	131.48	A(80,79,82)	109.42
A(37,1,65)	145.60	A(41,2,43)	63.88	A(13,17,20)	111.32	A(40,41,42)	121.88	A(64,63,68)	116.80	A(81,79,82)	106.88
A(37,1,66)	157.60	A(41,2,44)	75.54	A(18,17,19)	108.68	A(40,41,46)	118.98	A(64,63,73)	123.88	A(66,83,84)	111.67
A(37,1,67)	122.60	A(42,2,44)	64.84	A(18,17,20)	108.01	A(42,41,46)	119.13	A(68,63,73)	119.31	A(66,83,85)	109.51
A(37,1,68)	92.98	A(1,3,9)	117.10	A(19,17,20)	108.30	A(2,42,59)	130.26	A(1,64,69)	127.00	A(66,83,86)	111.72
A(63,1,65)	63.59	A(1,3,12)	124.50	A(16,21,22)	110.79	A(41,42,43)	116.31	A(63,64,65)	121.43	A(84,83,85)	107.65
A(63,1,66)	75.62	A(9,3,12)	117.94	A(16,21,23)	110.00	A(41,42,59)	122.26	A(63,64,69)	119.75	A(84,83,86)	108.70
A(63,1,67)	64.16	A(2,4,10)	124.50	A(16,21,24)	111.37	A(43,42,59)	121.41	A(65,64,69)	118.81	A(85,83,86)	107.42
A(64,1,66)	63.94	A(2,4,11)	117.10	A(22,21,23)	108.28	A(2,43,47)	122.99	A(1,65,70)	125.51		Cont...
A(64,1,67)	74.97	A(10,4,11)	117.94	A(22,21,24)	108.60	A(42,43,44)	121.86	A(64,65,66)	121.88		

A(64,1,68)	63.23	A(1,5,6)	113.59	A(23,21,24)	107.69	A(42,43,47)	119.00	A(64,65,70)	118.98		
A(65,1,67)	63.88	A(1,5,16)	139.49	A(8,25,26)	105.23	A(44,43,47)	119.09	A(66,65,70)	119.13		
A(65,1,68)	75.54	A(6,5,16)	106.45	A(8,25,29)	125.09	A(2,44,48)	123.66	A(1,66,83)	130.26		
A(66,1,68)	64.84	A(5,6,9)	116.34	A(26,25,29)	129.68	A(39,44,43)	121.29	A(65,66,67)	116.31		
A(4,2,7)	77.03	A(5,6,13)	110.96	A(25,26,27)	126.00	A(39,44,48)	119.07	A(65,66,83)	122.26		
A(4,2,38)	83.67	A(9,6,13)	132.68	A(25,26,28)	107.94	A(43,44,48)	119.64	A(67,66,83)	121.41		
A(4,2,39)	150.60	A(2,7,8)	113.59	A(27,26,28)	126.06	A(39,49,50)	106.40	A(1,67,71)	122.99		
A(4,2,40)	166.40	A(2,7,28)	139.49	A(7,28,26)	109.41	A(39,49,51)	114.64	A(66,67,68)	121.86		
A(4,2,41)	130.60	A(8,7,28)	106.45	A(7,28,33)	123.30	A(39,49,55)	108.06	A(66,67,71)	119.00		
A(4,2,42)	103.10	A(7,8,11)	116.34	A(26,28,33)	127.29	A(50,49,51)	107.96	A(68,67,71)	119.09		
A(4,2,43)	97.11	A(7,8,25)	110.96	A(25,29,30)	111.32	A(50,49,55)	108.13	A(1,68,72)	123.66		
A(4,2,44)	116.50	A(11,8,25)	132.68	A(25,29,31)	108.64	A(51,49,55)	111.35	A(63,68,67)	121.29		
A(7,2,38)	84.05	A(3,9,6)	115.21	A(25,29,32)	111.79	A(49,51,52)	112.22	A(63,68,72)	119.07		
A(7,2,39)	130.10	A(3,9,10)	124.34	A(30,29,31)	108.30	A(49,51,53)	109.23	A(67,68,72)	119.64		

* For the atomic indices refer to Figure S1

Table S9 Various dihedral angles (°) in optimised [1]²⁺.

Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value
D(5,1,3,9)	-7.9	D(37,1,64,69)	-62.4	D(43,2,4,10)	-27.6	D(38,2,42,59)	-135.2	D(5,6,13,14)	-0.4	D(5,16,21,24)	67.9
D(5,1,3,12)	-179.9	D(66,1,64,69)	141.0	D(43,2,4,11)	160.5	D(39,2,42,59)	-179.5	D(5,6,13,17)	179.3	D(14,16,21,22)	126.5
D(37,1,3,9)	77.4	D(67,1,64,69)	177.9	D(44,2,4,10)	4.4	D(40,2,42,59)	145.8	D(9,6,13,14)	177.7	D(14,16,21,23)	6.8
D(37,1,3,12)	-94.6	D(68,1,64,69)	-145.5	D(44,2,4,11)	-167.6	D(44,2,42,59)	-143.1	D(9,6,13,17)	-2.5	D(14,16,21,24)	-112.5
D(63,1,3,9)	151.9	D(3,1,65,70)	68.9	D(4,2,7,8)	-6.2	D(4,2,43,47)	12.7	D(2,7,8,11)	3.9	D(8,25,26,27)	-179.7
D(63,1,3,12)	-20.1	D(5,1,65,70)	-11.9	D(4,2,7,28)	-176.9	D(7,2,43,47)	88.3	D(2,7,8,25)	-174.6	D(8,25,26,28)	0.2
D(64,1,3,9)	-106.9	D(37,1,65,70)	-104.7	D(38,2,7,8)	78.6	D(38,2,43,47)	-74.3	D(28,7,8,11)	177.6	D(29,25,26,27)	0.1
D(64,1,3,12)	81.1	D(63,1,65,70)	-142.3	D(38,2,7,28)	-92.1	D(39,2,43,47)	-143.6	D(28,7,8,25)	-0.9	D(29,25,26,28)	179.9
D(65,1,3,9)	-99.0	D(67,1,65,70)	145.1	D(39,2,7,8)	161.0	D(40,2,43,47)	-178.6	D(2,7,28,26)	172.1	D(8,25,29,30)	-64.7
D(65,1,3,12)	89.1	D(68,1,65,70)	-178.4	D(39,2,7,28)	-9.7	D(41,2,43,47)	144.7	D(2,7,28,33)	-7.6	D(8,25,29,31)	176.2
D(66,1,3,9)	-124.3	D(3,1,66,83)	29.7	D(40,2,7,8)	-172.3	D(4,2,44,48)	50.7	D(8,7,28,26)	1.0	D(8,25,29,32)	56.2
D(66,1,3,12)	63.8	D(5,1,66,83)	-52.4	D(40,2,7,28)	17.0	D(7,2,44,48)	-111.2	D(8,7,28,33)	-178.7	D(26,25,29,30)	115.6
D(67,1,3,9)	-160.5	D(37,1,66,83)	135.2	D(41,2,7,8)	-135.9	D(38,2,44,48)	-33.8	D(7,8,11,4)	2.7	D(26,25,29,31)	-3.6
D(67,1,3,12)	27.6	D(63,1,66,83)	179.5	D(41,2,7,28)	53.4	D(40,2,44,48)	-144.6	D(7,8,11,12)	-178.2	D(26,25,29,32)	-123.5
D(68,1,3,9)	167.6	D(64,1,66,83)	-145.8	D(42,2,7,8)	-104.3	D(41,2,44,48)	179.1	D(25,8,11,4)	-179.2	D(25,26,28,7)	-0.7
D(68,1,3,12)	-4.4	D(68,1,66,83)	143.1	D(42,2,7,28)	85.0	D(42,2,44,48)	143.2	D(25,8,11,12)	-0.1	D(25,26,28,33)	179.0
D(3,1,5,6)	6.2	D(3,1,67,71)	-12.7	D(43,2,7,8)	-86.7	D(1,3,9,6)	8.4	D(7,8,25,26)	0.4	D(27,26,28,7)	179.2
D(3,1,5,16)	176.9	D(5,1,67,71)	-88.3	D(43,2,7,28)	102.6	D(1,3,9,10)	-172.6	D(7,8,25,29)	-179.3	D(27,26,28,33)	-1.2
D(37,1,5,6)	-78.6	D(37,1,67,71)	74.3	D(44,2,7,8)	157.2	D(12,3,9,6)	-179.1	D(11,8,25,26)	-177.7	D(7,28,33,34)	-67.9
D(37,1,5,16)	92.1	D(63,1,67,71)	143.6	D(44,2,7,28)	-13.6	D(12,3,9,10)	0.0	D(11,8,25,29)	2.5	D(7,28,33,35)	172.8
D(63,1,5,6)	-161.0	D(64,1,67,71)	178.6	D(4,2,39,49)	85.6	D(1,3,12,11)	171.9	D(3,9,10,4)	0.0	D(7,28,33,36)	53.1
D(63,1,5,16)	9.7	D(65,1,67,71)	-144.7	D(7,2,39,49)	-68.3	D(9,3,12,11)	0.0	D(6,9,10,4)	179.1	D(26,28,33,34)	112.5
D(64,1,5,6)	172.3	D(3,1,68,72)	-50.7	D(38,2,39,49)	12.2	D(2,4,10,9)	-171.9	D(4,11,12,3)	0.0	D(26,28,33,35)	-6.8
D(64,1,5,16)	-17.0	D(5,1,68,72)	111.2	D(41,2,39,49)	-147.7	D(11,4,10,9)	0.0	D(8,11,12,3)	-179.1	D(26,28,33,36)	-126.5
D(65,1,5,6)	135.9	D(37,1,68,72)	33.8	D(42,2,39,49)	176.8	D(2,4,11,8)	-8.4	D(6,13,14,15)	179.7	D(44,39,40,41)	4.0
D(65,1,5,16)	-53.4	D(64,1,68,72)	144.6	D(43,2,39,49)	140.1	D(2,4,11,12)	172.6	D(6,13,14,16)	-0.2	D(44,39,40,45)	-175.3

D(66,1,5,6)	104.3	D(65,1,68,72)	-179.1	D(4,2,40,45)	-122.1	D(10,4,11,8)	179.1	D(17,13,14,15)	-0.1	D(49,39,40,41)	-177.4
D(66,1,5,16)	-85.0	D(66,1,68,72)	-143.2	D(7,2,40,45)	-26.5	D(10,4,11,12)	0.0	D(17,13,14,16)	-179.9	D(49,39,40,45)	3.3
D(67,1,5,6)	86.7	D(7,2,4,10)	179.9	D(38,2,40,45)	62.4	D(1,5,6,9)	-3.9	D(6,13,17,18)	-56.2	D(40,39,44,43)	-5.9
D(67,1,5,16)	-102.6	D(7,2,4,11)	7.9	D(42,2,40,45)	-141.0	D(1,5,6,13)	174.6	D(6,13,17,19)	-176.2	D(40,39,44,48)	173.8
D(68,1,5,6)	-157.2	D(38,2,4,10)	94.6	D(43,2,40,45)	-177.9	D(16,5,6,9)	-177.6	D(6,13,17,20)	64.7	D(49,39,44,43)	175.4
D(68,1,5,16)	13.6	D(38,2,4,11)	-77.4	D(44,2,40,45)	145.5	D(16,5,6,13)	0.9	D(14,13,17,18)	123.5	D(49,39,44,48)	-4.9
D(3,1,63,73)	-85.6	D(39,2,4,10)	20.1	D(4,2,41,46)	-68.9	D(1,5,16,14)	-172.1	D(14,13,17,19)	3.6	D(2,39,49,50)	-47.9
D(5,1,63,73)	68.3	D(39,2,4,11)	-151.9	D(7,2,41,46)	11.9	D(1,5,16,21)	7.6	D(14,13,17,20)	-115.6	D(2,39,49,51)	71.3
D(37,1,63,73)	-12.2	D(40,2,4,10)	-81.1	D(38,2,41,46)	104.7	D(6,5,16,14)	-1.0	D(13,14,16,5)	0.7	D(2,39,49,55)	-163.9
D(65,1,63,73)	147.7	D(40,2,4,11)	106.9	D(39,2,41,46)	142.3	D(6,5,16,21)	178.7	D(13,14,16,21)	-179.0	D(40,39,49,50)	-141.4
D(66,1,63,73)	-176.8	D(41,2,4,10)	-89.1	D(43,2,41,46)	-145.1	D(5,6,9,3)	-2.7	D(15,14,16,5)	-179.2	D(40,39,49,51)	-22.2
D(67,1,63,73)	-140.1	D(41,2,4,11)	99.0	D(44,2,41,46)	178.4	D(5,6,9,10)	178.2	D(15,14,16,21)	1.2	D(40,39,49,55)	102.6
D(3,1,64,69)	122.1	D(42,2,4,10)	-63.8	D(4,2,42,59)	-29.7	D(13,6,9,3)	179.2	D(5,16,21,22)	-53.1	D(44,39,49,50)	37.1
D(5,1,64,69)	26.5	D(42,2,4,11)	124.3	D(7,2,42,59)	52.4	D(13,6,9,10)	0.1	D(5,16,21,23)	-172.8	D(44,39,49,51)	156.4
D(44,39,49,55)	-78.8	D(50,49,55,58)	179.9	D(67,66,83,85)	-84.9	D(63,73,75,78)	-56.1	D(47,43,44,39)	179.3	D(69,64,65,70)	-0.2
D(39,40,41,42)	2.0	D(51,49,55,56)	-177.2	D(67,66,83,86)	34.0	D(74,73,75,76)	-179.9	D(47,43,44,48)	-0.4	D(64,65,66,67)	6.1
D(39,40,41,46)	-179.1	D(51,49,55,57)	-57.7	D(66,67,68,63)	-1.9	D(74,73,75,77)	-60.8	D(39,49,51,52)	65.5	D(64,65,66,83)	-175.3
D(45,40,41,42)	-178.6	D(51,49,55,58)	61.4	D(66,67,68,72)	177.8	D(74,73,75,78)	58.7	D(39,49,51,53)	-176.1	D(70,65,66,67)	-175.1
D(45,40,41,46)	0.2	D(68,63,64,65)	-4.0	D(71,67,68,63)	-179.3	D(79,73,75,76)	-61.4	D(39,49,51,54)	-57.5	D(70,65,66,83)	3.6
D(40,41,42,43)	-6.1	D(68,63,64,69)	175.3	D(71,67,68,72)	0.4	D(79,73,75,77)	57.7	D(50,49,51,52)	-176.1	D(65,66,67,68)	-4.1
D(40,41,42,59)	175.3	D(73,63,64,65)	177.4	D(63,73,75,76)	65.3	D(79,73,75,78)	177.2	D(50,49,51,53)	-57.7	D(65,66,67,71)	173.3
D(46,41,42,43)	175.1	D(73,63,64,69)	-3.3	D(63,73,75,77)	-175.6	D(63,73,79,80)	57.5	D(50,49,51,54)	60.9	D(83,66,67,68)	177.2
D(46,41,42,59)	-3.6	D(64,63,68,67)	5.9	D(75,73,79,80)	-179.4	D(63,73,79,81)	176.1	D(55,49,51,52)	-57.5	D(83,66,67,71)	-5.3
D(41,42,43,44)	4.1	D(64,63,68,72)	-173.8	D(75,73,79,81)	-60.8	D(63,73,79,82)	-65.5	D(55,49,51,53)	60.8	D(1,66,83,84)	68.2
D(41,42,43,47)	-173.3	D(73,63,68,67)	-175.4	D(75,73,79,82)	57.5	D(74,73,79,80)	-60.9	D(55,49,51,54)	179.4	D(1,66,83,85)	-172.7
D(59,42,43,44)	-177.2	D(73,63,68,72)	4.9	D(64,63,73,74)	141.4	D(74,73,79,81)	57.7	D(39,49,55,56)	56.1	D(1,66,83,86)	-53.8
D(59,42,43,47)	5.3	D(1,63,73,74)	47.9	D(64,63,73,75)	-102.6	D(74,73,79,82)	176.1	D(39,49,55,57)	175.6	D(65,66,83,84)	-22.6
D(2,42,59,60)	-68.2	D(1,63,73,75)	163.9	D(64,63,73,79)	22.2	D(50,49,55,57)	60.8	D(39,49,55,58)	-65.3	D(65,66,83,85)	96.5
D(2,42,59,61)	53.8	D(1,63,73,79)	-71.3	D(68,63,73,74)	-37.1	D(67,66,83,84)	156.0	D(50,49,55,56)	-58.7	D(65,66,83,86)	-144.6

D(2,42,59,62)	172.7	D(68,63,73,75)	78.8	D(63,64,65,70)	179.1	D(41,42,59,62)	-96.5	D(43,42,59,61)	-34.0	D(42,43,44,39)	1.9
D(41,42,59,60)	22.6	D(68,63,73,79)	-156.4	D(69,64,65,66)	178.6	D(43,42,59,60)	-156.0	D(43,42,59,62)	84.9	D(42,43,44,48)	-177.8

* For the atomic indices refer to Figure S1

Fig. S3 Pictorial representations of important Kohn-Sham molecular orbitals of [1].

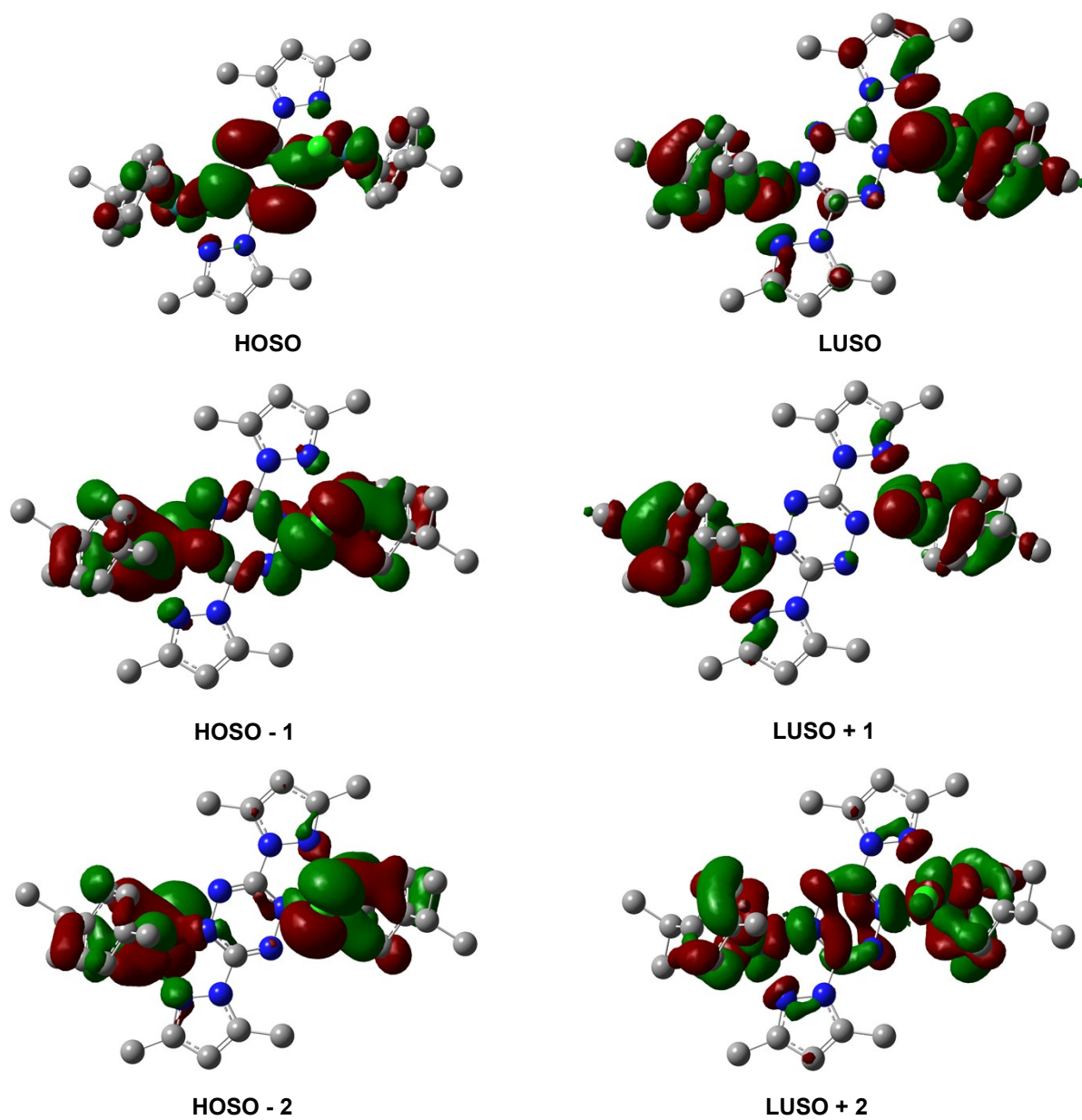


Table S10 Calculated energies of Kohn-Sham molecular orbitals (MO) at the B3LYP Level and the contributions of various molecular groups to the MOs of [1].

Sr. No.	MO's	Energy(eV)	Contribution of the group to MO (%)			
			bpytz	Cl	Ru	p-cym
189	LUMO+10	0.78	5	0	88	7
188	LUMO+9	0.21	63	0	15	21
187	LUMO+8	0.07	8	0	32	60
186	LUMO+7	0.01	6	1	26	67
185	LUMO+6	-0.07	9	2	21	67
184	LUMO+5	-0.27	30	1	12	57
183	LUMO+4	-0.55	31	2	36	32
182	LUMO+3	-0.67	78	0	9	12
181	LUMO+2	-0.83	19	2	51	28
180	LUMO+1	-0.95	6	11	50	32
179	LUMO	-0.98	12	11	46	31
178	HOMO	-3.4	76	0	16	8
177	HOMO-1	-5	16	24	44	15
176	HOMO-2	-5.14	6	35	42	17
175	HOMO-3	-5.28	12	30	47	11
174	HOMO-4	-5.47	13	40	41	7
173	HOMO-5	-5.88	8	35	44	12
172	HOMO-6	-5.9	9	29	48	13
171	HOMO-7	-6.05	63	29	8	1
170	HOMO-8	-6.31	48	31	19	3
169	HOMO-9	-6.38	40	27	30	3
168	HOMO-10	-6.41	74	12	12	3

Table S11 Bond lengths (Å) of optimised [1].

Definition*	Value	Definition*	Value	Definition*	Value
R(1,3)	2.0669	R(21,22)	1.0941	R(63,73)	1.517
R(1,5)	2.1108	R(21,23)	1.0927	R(64,65)	1.4353
R(1,37)	2.4326	R(21,24)	1.0963	R(64,69)	1.0823
R(1,63)	2.3494	R(25,26)	1.3777	R(65,66)	1.4136
R(1,64)	2.3233	R(25,29)	1.4926	R(65,70)	1.0857
R(1,65)	2.2645	R(26,27)	1.0803	R(66,67)	1.4348
R(1,66)	2.3045	R(26,28)	1.4138	R(66,83)	1.5046
R(1,67)	2.2405	R(28,33)	1.4947	R(67,68)	1.4078
R(1,68)	2.2537	R(29,30)	1.0947	R(67,71)	1.0844
R(2,4)	2.0669	R(29,31)	1.0929	R(68,72)	1.084
R(2,7)	2.1108	R(29,32)	1.0937	R(73,74)	1.0967
R(2,38)	2.4326	R(33,34)	1.0963	R(73,75)	1.546
R(2,39)	2.3494	R(33,35)	1.0927	R(73,79)	1.5331
R(2,40)	2.3233	R(33,36)	1.0941	R(75,76)	1.0963
R(2,41)	2.2645	R(39,40)	1.406	R(75,77)	1.0949
R(2,42)	2.3045	R(39,44)	1.441	R(75,78)	1.0957
R(2,43)	2.2405	R(39,49)	1.517	R(79,80)	1.0945
R(2,44)	2.2537	R(40,41)	1.4353	R(79,81)	1.0945
R(3,9)	1.3465	R(40,45)	1.0823	R(79,82)	1.0971
R(3,12)	1.3690	R(41,42)	1.4136	R(83,84)	1.0937
R(4,10)	1.3690	R(41,46)	1.0857	R(83,85)	1.0974
R(4,11)	1.3465	R(42,43)	1.4348	R(83,86)	1.0943
R(5,6)	1.3749	R(42,59)	1.5046		
R(5,16)	1.3324	R(43,44)	1.4078		
R(6,9)	1.3981	R(43,47)	1.0844		
R(6,13)	1.3778	R(44,48)	1.084		
R(7,8)	1.3749	R(49,50)	1.0967		
R(7,28)	1.3324	R(49,51)	1.5331		
R(8,11)	1.3981	R(49,55)	1.546		
R(8,25)	1.3778	R(51,52)	1.0971		
R(9,10)	1.3166	R(51,53)	1.0945		
R(11,12)	1.3166	R(51,54)	1.0945		
R(13,14)	1.3777	R(55,56)	1.0957		
R(13,17)	1.4926	R(55,57)	1.0949		
R(14,15)	1.0803	R(55,58)	1.0963		
R(14,16)	1.4138	R(59,60)	1.0937		
R(16,21)	1.4947	R(59,61)	1.0943		
R(17,18)	1.0937	R(59,62)	1.0974		
R(17,19)	1.0929	R(63,64)	1.406		
R(17,20)	1.0947	R(63,68)	1.441		

Table S12 Bond angles (°) of optimised [1].

Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value
A(3,1,5)	75.74	A(7,2,40)	105.45	A(6,9,10)	119.01	A(30,29,32)	107.48	A(49,51,54)	110.98	A(63,73,74)	106.11
A(3,1,37)	84.31	A(7,2,41)	98.31	A(4,10,9)	114.85	A(31,29,32)	109.12	A(52,51,53)	106.99	A(63,73,75)	108.79
A(3,1,63)	151.34	A(7,2,42)	116.18	A(4,11,8)	113.96	A(28,33,34)	111.54	A(52,51,54)	109.38	A(63,73,79)	114.47
A(3,1,64)	163.31	A(7,2,43)	150.43	A(4,11,12)	127.03	A(28,33,35)	109.96	A(53,51,54)	107.71	A(74,73,75)	108.33
A(3,1,65)	127.02	A(7,2,44)	168.04	A(8,11,12)	119.01	A(28,33,36)	110.84	A(49,55,56)	112.00	A(74,73,79)	107.46
A(3,1,66)	99.07	A(38,2,39)	89.87	A(3,12,11)	114.85	A(34,33,35)	107.70	A(49,55,57)	109.74	A(75,73,79)	111.37
A(3,1,67)	94.57	A(38,2,40)	112.37	A(6,13,14)	105.55	A(34,33,36)	108.32	A(49,55,58)	111.12	A(73,75,76)	111.12
A(3,1,68)	115.97	A(38,2,41)	148.36	A(6,13,17)	125.26	A(35,33,36)	108.36	A(56,55,57)	107.86	A(73,75,77)	109.74
A(5,1,37)	84.24	A(38,2,42)	159.54	A(14,13,17)	129.19	A(2,39,49)	130.54	A(56,55,58)	108.01	A(73,75,78)	112.00
A(5,1,63)	131.64	A(38,2,43)	123.12	A(13,14,15)	126.07	A(40,39,44)	117.24	A(57,55,58)	107.97	A(76,75,77)	107.97
A(5,1,64)	105.45	A(38,2,44)	94.25	A(13,14,16)	107.45	A(40,39,49)	123.83	A(42,59,60)	111.41	A(76,75,78)	108.01
A(5,1,65)	98.31	A(39,2,41)	64.81	A(15,14,16)	126.48	A(44,39,49)	118.92	A(42,59,61)	111.26	A(77,75,78)	107.86
A(5,1,66)	116.18	A(39,2,42)	77.46	A(5,16,14)	109.34	A(2,40,45)	127.20	A(42,59,62)	110.13	A(73,79,80)	110.98
A(5,1,67)	150.43	A(39,2,43)	65.43	A(5,16,21)	122.95	A(39,40,41)	121.06	A(60,59,61)	108.37	A(73,79,81)	109.40
A(5,1,68)	168.04	A(40,2,42)	65.17	A(14,16,21)	127.71	A(39,40,45)	119.94	A(60,59,62)	107.79	A(73,79,82)	112.21
A(37,1,63)	89.87	A(40,2,43)	76.17	A(13,17,18)	111.68	A(41,40,45)	118.92	A(61,59,62)	107.74	A(80,79,81)	107.71
A(37,1,64)	112.37	A(40,2,44)	64.13	A(13,17,19)	108.72	A(2,41,46)	125.34	A(1,63,73)	130.54	A(80,79,82)	109.38
A(37,1,65)	148.36	A(41,2,43)	65.00	A(13,17,20)	111.20	A(40,41,42)	122.06	A(64,63,68)	117.24	A(81,79,82)	106.99
A(37,1,66)	159.54	A(41,2,44)	76.80	A(18,17,19)	109.12	A(40,41,46)	118.95	A(64,63,73)	123.83	A(66,83,84)	111.41
A(37,1,67)	123.12	A(42,2,44)	66.04	A(18,17,20)	107.48	A(42,41,46)	118.99	A(68,63,73)	118.92	A(66,83,85)	110.13
A(37,1,68)	94.25	A(1,3,9)	118.35	A(19,17,20)	108.57	A(2,42,59)	129.29	A(1,64,69)	127.20	A(66,83,86)	111.26
A(63,1,65)	64.81	A(1,3,12)	122.90	A(16,21,22)	110.84	A(41,42,43)	116.37	A(63,64,65)	121.06	A(84,83,85)	107.79
A(63,1,66)	77.46	A(9,3,12)	118.13	A(16,21,23)	109.96	A(41,42,59)	122.40	A(63,64,69)	119.94	A(84,83,86)	108.37
A(63,1,67)	65.43	A(2,4,10)	122.90	A(16,21,24)	111.54	A(43,42,59)	121.21	A(65,64,69)	118.92	A(85,83,86)	107.74
A(64,1,66)	65.17	A(2,4,11)	118.35	A(22,21,23)	108.36	A(2,43,47)	122.23	A(1,65,70)	125.34		
A(64,1,67)	76.17	A(10,4,11)	118.13	A(22,21,24)	108.32	A(42,43,44)	121.83	A(64,65,66)	122.06		

A(64,1,68)	64.13	A(1,5,6)	114.36	A(23,21,24)	107.70	A(42,43,47)	118.92	A(64,65,70)	118.95		
A(65,1,67)	65.00	A(1,5,16)	138.70	A(8,25,26)	105.55	A(44,43,47)	119.06	A(66,65,70)	118.99		
A(65,1,68)	76.80	A(6,5,16)	106.62	A(8,25,29)	125.26	A(2,44,48)	123.52	A(1,66,83)	129.29		
A(66,1,68)	66.04	A(5,6,9)	116.75	A(26,25,29)	129.19	A(39,44,43)	121.24	A(65,66,67)	116.37		
A(4,2,7)	75.74	A(5,6,13)	111.03	A(25,26,27)	126.07	A(39,44,48)	119.12	A(65,66,83)	122.40		
A(4,2,38)	84.31	A(9,6,13)	132.20	A(25,26,28)	107.45	A(43,44,48)	119.59	A(67,66,83)	121.21		
A(4,2,39)	151.34	A(2,7,8)	114.36	A(27,26,28)	126.48	A(39,49,50)	106.11	A(1,67,71)	122.23		
A(4,2,40)	163.31	A(2,7,28)	138.70	A(7,28,26)	109.34	A(39,49,51)	114.47	A(66,67,68)	121.83		
A(4,2,41)	127.02	A(8,7,28)	106.62	A(7,28,33)	122.95	A(39,49,55)	108.79	A(66,67,71)	118.92		
A(4,2,42)	99.07	A(7,8,11)	116.75	A(26,28,33)	127.71	A(50,49,51)	107.46	A(68,67,71)	119.06		
A(4,2,43)	94.57	A(7,8,25)	111.03	A(25,29,30)	111.20	A(50,49,55)	108.33	A(1,68,72)	123.52		
A(4,2,44)	115.97	A(11,8,25)	132.20	A(25,29,31)	108.72	A(51,49,55)	111.37	A(63,68,67)	121.24		
A(7,2,38)	84.24	A(3,9,6)	113.96	A(25,29,32)	111.68	A(49,51,52)	112.21	A(63,68,72)	119.12		
A(7,2,39)	131.64	A(3,9,10)	127.03	A(30,29,31)	108.57	A(49,51,53)	109.40	A(67,68,72)	119.59		

* For the atomic indices refer to Figure S1

Table S13 Various dihedral angles (°) in optimised [1]

Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value	Definition*	Value
D(5,1,3,9)	-8.5	D(37,1,64,69)	-61.7	D(43,2,4,10)	-29.1	D(38,2,42,59)	-126.5	D(5,6,13,14)	-0.3	D(5,16,21,24)	69.5
D(5,1,3,12)	-179.3	D(66,1,64,69)	140.5	D(43,2,4,11)	160.2	D(39,2,42,59)	-179.5	D(5,6,13,17)	179.5	D(14,16,21,22)	128.2
D(37,1,3,9)	77.0	D(67,1,64,69)	177.9	D(44,2,4,10)	1.8	D(40,2,42,59)	145.8	D(9,6,13,14)	178.3	D(14,16,21,23)	8.4
D(37,1,3,12)	-93.8	D(68,1,64,69)	-145.3	D(44,2,4,11)	-168.9	D(44,2,42,59)	-142.9	D(9,6,13,17)	-1.8	D(14,16,21,24)	-111.0
D(63,1,3,9)	156.2	D(3,1,65,70)	68.7	D(4,2,7,8)	-6.1	D(4,2,43,47)	15.4	D(2,7,8,11)	3.4	D(8,25,26,27)	-179.8
D(63,1,3,12)	-14.6	D(5,1,65,70)	-9.7	D(4,2,7,28)	-178.5	D(7,2,43,47)	84.4	D(2,7,8,25)	-175.4	D(8,25,26,28)	0.1
D(64,1,3,9)	-104.8	D(37,1,65,70)	-102.2	D(38,2,7,8)	79.5	D(38,2,43,47)	-70.8	D(28,7,8,11)	178.2	D(29,25,26,27)	0.0
D(64,1,3,12)	84.5	D(63,1,65,70)	-142.0	D(38,2,7,28)	-92.9	D(39,2,43,47)	-143.2	D(28,7,8,25)	-0.7	D(29,25,26,28)	180.0
D(65,1,3,9)	-98.2	D(67,1,65,70)	144.7	D(39,2,7,8)	164.1	D(40,2,43,47)	-178.7	D(2,7,28,26)	173.5	D(8,25,29,30)	-65.3
D(65,1,3,12)	91.0	D(68,1,65,70)	-178.6	D(39,2,7,28)	-8.2	D(41,2,43,47)	144.4	D(2,7,28,33)	-6.1	D(8,25,29,31)	175.2
D(66,1,3,9)	-123.4	D(3,1,66,83)	28.4	D(40,2,7,8)	-168.9	D(4,2,44,48)	54.2	D(8,7,28,26)	0.8	D(8,25,29,32)	54.8
D(66,1,3,12)	65.9	D(5,1,66,83)	-50.1	D(40,2,7,28)	18.7	D(7,2,44,48)	-113.8	D(8,7,28,33)	-178.8	D(26,25,29,30)	114.9
D(67,1,3,9)	-160.2	D(37,1,66,83)	126.5	D(41,2,7,8)	-132.3	D(38,2,44,48)	-31.5	D(7,8,11,4)	3.6	D(26,25,29,31)	-4.6
D(67,1,3,12)	29.1	D(63,1,66,83)	179.5	D(41,2,7,28)	55.3	D(40,2,44,48)	-144.4	D(7,8,11,12)	-177.0	D(26,25,29,32)	-125.1
D(68,1,3,9)	168.9	D(64,1,66,83)	-145.8	D(42,2,7,8)	-99.4	D(41,2,44,48)	179.2	D(25,8,11,4)	-177.8	D(25,26,28,7)	-0.6
D(68,1,3,12)	-1.8	D(68,1,66,83)	142.9	D(42,2,7,28)	88.3	D(42,2,44,48)	142.8	D(25,8,11,12)	1.6	D(25,26,28,33)	179.0
D(3,1,5,6)	6.1	D(3,1,67,71)	-15.4	D(43,2,7,8)	-79.8	D(1,3,9,6)	9.3	D(7,8,25,26)	0.3	D(27,26,28,7)	179.4
D(3,1,5,16)	178.5	D(5,1,67,71)	-84.4	D(43,2,7,28)	107.8	D(1,3,9,10)	-171.3	D(7,8,25,29)	-179.5	D(27,26,28,33)	-1.0
D(37,1,5,6)	-79.5	D(37,1,67,71)	70.8	D(44,2,7,8)	162.7	D(12,3,9,6)	-179.5	D(11,8,25,26)	-178.3	D(7,28,33,34)	-69.5
D(37,1,5,16)	92.9	D(63,1,67,71)	143.2	D(44,2,7,28)	-9.6	D(12,3,9,10)	-0.2	D(11,8,25,29)	1.8	D(7,28,33,35)	171.1
D(63,1,5,6)	-164.1	D(64,1,67,71)	178.7	D(4,2,39,49)	90.5	D(1,3,12,11)	170.9	D(3,9,10,4)	0.1	D(7,28,33,36)	51.3
D(63,1,5,16)	8.2	D(65,1,67,71)	-144.4	D(7,2,39,49)	-69.5	D(9,3,12,11)	0.1	D(6,9,10,4)	179.5	D(26,28,33,34)	111.0
D(64,1,5,6)	168.9	D(3,1,68,72)	-54.2	D(38,2,39,49)	12.7	D(2,4,10,9)	-170.9	D(4,11,12,3)	-0.1	D(26,28,33,35)	-8.4
D(64,1,5,16)	-18.7	D(5,1,68,72)	113.8	D(41,2,39,49)	-147.7	D(11,4,10,9)	-0.1	D(8,11,12,3)	-179.5	D(26,28,33,36)	-128.2
D(65,1,5,6)	132.3	D(37,1,68,72)	31.5	D(42,2,39,49)	176.5	D(2,4,11,8)	-9.3	D(6,13,14,15)	179.8	D(44,39,40,41)	0.7

D(65,1,5,16)	-55.3	D(64,1,68,72)	144.4	D(43,2,39,49)	139.7	D(2,4,11,12)	171.3	D(6,13,14,16)	-0.1	D(44,39,40,45)	-176.0
D(66,1,5,6)	99.4	D(65,1,68,72)	-179.2	D(4,2,40,45)	-120.2	D(10,4,11,8)	179.5	D(17,13,14,15)	0.0	D(49,39,40,41)	179.8
D(66,1,5,16)	-88.3	D(66,1,68,72)	-142.8	D(7,2,40,45)	-28.4	D(10,4,11,12)	0.2	D(17,13,14,16)	-180.0	D(49,39,40,45)	3.1
D(67,1,5,6)	79.8	D(7,2,4,10)	179.3	D(38,2,40,45)	61.7	D(1,5,6,9)	-3.4	D(6,13,17,18)	-54.8	D(40,39,44,43)	-3.1
D(67,1,5,16)	-107.8	D(7,2,4,11)	8.5	D(42,2,40,45)	-140.5	D(1,5,6,13)	175.4	D(6,13,17,19)	-175.2	D(40,39,44,48)	174.3
D(68,1,5,6)	-162.7	D(38,2,4,10)	93.8	D(43,2,40,45)	-177.9	D(16,5,6,9)	-178.2	D(6,13,17,20)	65.3	D(49,39,44,43)	177.8
D(68,1,5,16)	9.6	D(38,2,4,11)	-77.0	D(44,2,40,45)	145.3	D(16,5,6,13)	0.7	D(14,13,17,18)	125.1	D(49,39,44,48)	-4.8
D(3,1,63,73)	-90.5	D(39,2,4,10)	14.6	D(4,2,41,46)	-68.7	D(1,5,16,14)	-173.5	D(14,13,17,19)	4.6	D(2,39,49,50)	-48.1
D(5,1,63,73)	69.5	D(39,2,4,11)	-156.2	D(7,2,41,46)	9.7	D(1,5,16,21)	6.1	D(14,13,17,20)	-114.9	D(2,39,49,51)	70.2
D(37,1,63,73)	-12.7	D(40,2,4,10)	-84.5	D(38,2,41,46)	102.2	D(6,5,16,14)	-0.8	D(13,14,16,5)	0.6	D(2,39,49,55)	-164.5
D(65,1,63,73)	147.7	D(40,2,4,11)	104.8	D(39,2,41,46)	142.0	D(6,5,16,21)	178.8	D(13,14,16,21)	-179.0	D(40,39,49,50)	-142.1
D(66,1,63,73)	-176.5	D(41,2,4,10)	-91.0	D(43,2,41,46)	-144.7	D(5,6,9,3)	-3.6	D(15,14,16,5)	-179.4	D(40,39,49,51)	-23.8
D(67,1,63,73)	-139.7	D(41,2,4,11)	98.2	D(44,2,41,46)	178.6	D(5,6,9,10)	177.0	D(15,14,16,21)	1.0	D(40,39,49,55)	101.5
D(3,1,64,69)	120.2	D(42,2,4,10)	-65.9	D(4,2,42,59)	-28.4	D(13,6,9,3)	177.8	D(5,16,21,22)	-51.3	D(44,39,49,50)	36.9
D(5,1,64,69)	28.4	D(42,2,4,11)	123.4	D(7,2,42,59)	50.1	D(13,6,9,10)	-1.6	D(5,16,21,23)	-171.1	D(44,39,49,51)	155.3
D(44,39,49,55)	-79.4	D(50,49,55,58)	179.7	D(67,66,83,85)	-82.8	D(47,43,44,39)	176.4	D(69,64,65,70)	-0.1	D(55,49,51,52)	-58.5
D(39,40,41,42)	3.5	D(51,49,55,56)	-177.4	D(67,66,83,86)	36.6	D(47,43,44,48)	-1.0	D(64,65,66,67)	5.0	D(55,49,51,53)	60.1
D(39,40,41,46)	-176.6	D(51,49,55,57)	-57.6	D(66,67,68,63)	-1.4	D(39,49,51,52)	65.4	D(64,65,66,83)	-176.8	D(55,49,51,54)	178.8
D(45,40,41,42)	-179.8	D(51,49,55,58)	61.7	D(66,67,68,72)	176.0	D(39,49,51,53)	-176.0	D(70,65,66,67)	-175.1	D(39,49,55,56)	55.5
D(45,40,41,46)	0.1	D(68,63,64,65)	-0.7	D(71,67,68,63)	-176.4	D(39,49,51,54)	-57.3	D(70,65,66,83)	3.1	D(39,49,55,57)	175.3
D(40,41,42,43)	-5.0	D(68,63,64,69)	176.0	D(71,67,68,72)	1.0	D(50,49,51,52)	-177.0	D(65,66,67,68)	-2.6	D(39,49,55,58)	-65.4
D(40,41,42,59)	176.8	D(73,63,64,65)	-179.8	D(63,73,75,76)	65.4	D(50,49,51,53)	-58.4	D(65,66,67,71)	172.4	D(50,49,55,56)	-59.4
D(46,41,42,43)	175.1	D(73,63,64,69)	-3.1	D(63,73,75,77)	-175.3	D(50,49,51,54)	60.3	D(83,66,67,68)	179.2	D(50,49,55,57)	60.4
D(46,41,42,59)	-3.1	D(64,63,68,67)	3.1	D(42,43,44,39)	1.4	D(63,73,75,78)	-55.5	D(63,73,79,81)	176.0	D(83,66,67,71)	-5.8
D(41,42,43,44)	2.6	D(64,63,68,72)	-174.3	D(42,43,44,48)	-176.0	D(74,73,75,76)	-179.7	D(63,73,79,82)	-65.4	D(1,66,83,84)	70.0
D(41,42,43,47)	-172.4	D(73,63,68,67)	-177.8	D(68,63,73,74)	-36.9	D(74,73,75,77)	-60.4	D(74,73,79,80)	-60.3	D(1,66,83,85)	-170.4
D(59,42,43,44)	-179.2	D(73,63,68,72)	4.8	D(68,63,73,75)	79.4	D(74,73,75,78)	59.4	D(74,73,79,81)	58.4	D(1,66,83,86)	-51.1
D(59,42,43,47)	5.8	D(1,63,73,74)	48.1	D(68,63,73,79)	-155.3	D(79,73,75,76)	-61.7	D(74,73,79,82)	177.0	D(65,66,83,84)	-20.4
D(2,42,59,60)	-70.0	D(1,63,73,75)	164.5	D(63,64,65,66)	-3.5	D(79,73,75,77)	57.6	D(75,73,79,80)	-178.8	D(65,66,83,85)	99.2

D(2,42,59,61)	51.1	D(1,63,73,79)	-70.2	D(63,64,65,70)	176.6	D(79,73,75,78)	177.4	D(75,73,79,81)	-60.1	D(65,66,83,86)	-141.5
D(2,42,59,62)	170.4	D(64,63,73,74)	142.1	D(69,64,65,66)	179.8	D(63,73,79,80)	57.3	D(75,73,79,82)	58.5	D(67,66,83,84)	157.6
D(41,42,59,60)	20.4	D(64,63,73,75)	-101.5	D(41,42,59,62)	-99.2	D(43,42,59,61)	-36.6				
D(41,42,59,61)	141.5	D(64,63,73,79)	23.8	D(43,42,59,60)	-157.6	D(43,42,59,62)	82.8				

* For the atomic indices refer to Figure S1

Table S14. TD-DFT calculated electronic transitions for $[1]^+$, $[1]^{2+}$, and $[1]$.

State	λ/nm (Expt.)	λ/nm (DFT)	Oscillator Strength (<i>f</i>)	Transition*	Character
$[1]^+$	491	466	0.037	176 α \rightarrow 180 α (-0.3) 175 β \rightarrow 178 β (0.63) 176 β \rightarrow 180 β (-0.3)	Ru(d π)/ <i>p</i> -cym(π)/Cl(p π) \rightarrow Ru(d π)/ <i>p</i> -cym(π^*)/Ru-Cl(σ^*) Ru(d π)/bpytz(π)/Cl(p π) \rightarrow bpytz(π^*)
	491	502	0.042	175 β \rightarrow 178 β (0.5) 177 β \rightarrow 178 β (0.5)	Ru(d π)/ <i>p</i> -cym(π)/Cl(p π) \rightarrow Ru(d π)/ <i>p</i> -cym(π^*)/Ru-Cl(σ^*) Ru(d π)/bpytz(π)/Cl(p π) \rightarrow bpytz(π^*) Ru(d π)/ <i>p</i> -cym(π)/Cl(p π) \rightarrow bpytz(π^*)
$[1]^{2+}$	n.o.	501	0.021	169 \rightarrow 178(-0.3) 171 \rightarrow 178(0.6)	Ru(d π)/bpytz(π)/Cl(p π) \rightarrow Ru(d π)/bpytz(π^*) Cl(p π)/bpytz(π) \rightarrow Ru(d π)/bpytz(π^*)
	n.o.	600	0.042	173 \rightarrow 178(0.7)	<i>p</i> -cym(π)/Cl(p π) \rightarrow Ru(d π)/bpytz(π^*)
	716	752	0.170	175 \rightarrow 178(0.6) 177 \rightarrow 178(-0.3)	Ru(d π)/bpytz(π)/Cl(p π) \rightarrow Ru(d π)/bpytz(π^*) (<i>p</i> -cym(π)/Cl(p π)/bpytz(π) \rightarrow (Ru(d π)/bpytz(π^*))
$[1]$	450	473	0.030	176 \rightarrow 180(-0.4) 177 \rightarrow 179(0.4)	Ru(d π)/bpytz(π)/ <i>p</i> -cym(π)/Cl(p π) \rightarrow Ru(d π)/bpytz(π^*)/ <i>p</i> -cym(π^*)/Ru-Cl(σ^*) Ru(d π)/bpytz(π)/ <i>p</i> -cym(π)/Cl(p π) \rightarrow Ru(d π)/bpytz(π^*)/ <i>p</i> -cym(π^*)/Ru-Cl(σ^*)
	450	500			
	n.o.	652	0.067	178 \rightarrow 184(0.7)	bpytz(π)/ <i>p</i> -cym(π) \rightarrow bpytz(π^*)/ <i>p</i> -cym(π^*)
	n.o.	653	0.148	178 \rightarrow 181(0.6) 178 \rightarrow 182(-0.3)	bpytz(π)/ <i>p</i> -cym(π) \rightarrow bpytz(π^*)/ <i>p</i> -cym(π^*)/Ru(d π) bpytz(π)/ <i>p</i> -cym(π) \rightarrow bpytz(π^*)/ <i>p</i> -cym(π^*)/Ru(d π)
			0.037	178 \rightarrow 181(0.3) 178 \rightarrow 182(0.6)	bpytz(π)/ <i>p</i> -cym(π) \rightarrow bpytz(π^*)/ <i>p</i> -cym(π^*)/Ru(d π) bpytz(π)/ <i>p</i> -cym(π) \rightarrow bpytz(π^*)/ <i>p</i> -cym(π^*)/Ru(d π)

*HOMO of $[1]^+$, $[1]^{2+}$, $[1]$ are 178 α , 177, 178 respectively. Here, “n.o.” indicates that the band was not observed.

Fig. S4 Experimental and theoretical UV-vis-NIR spectra of the native [1]⁺, oxidised [1]²⁺ and reduced [1] species.

