Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Electronic Supporting Information

Oxidovanadium(IV), Oxidomolybdenum(VI) and Cobalt(III) Complexes of o-Phenylenediamine Derivatives: Oxidative Dehydrogenation and Photoluminescence

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Content

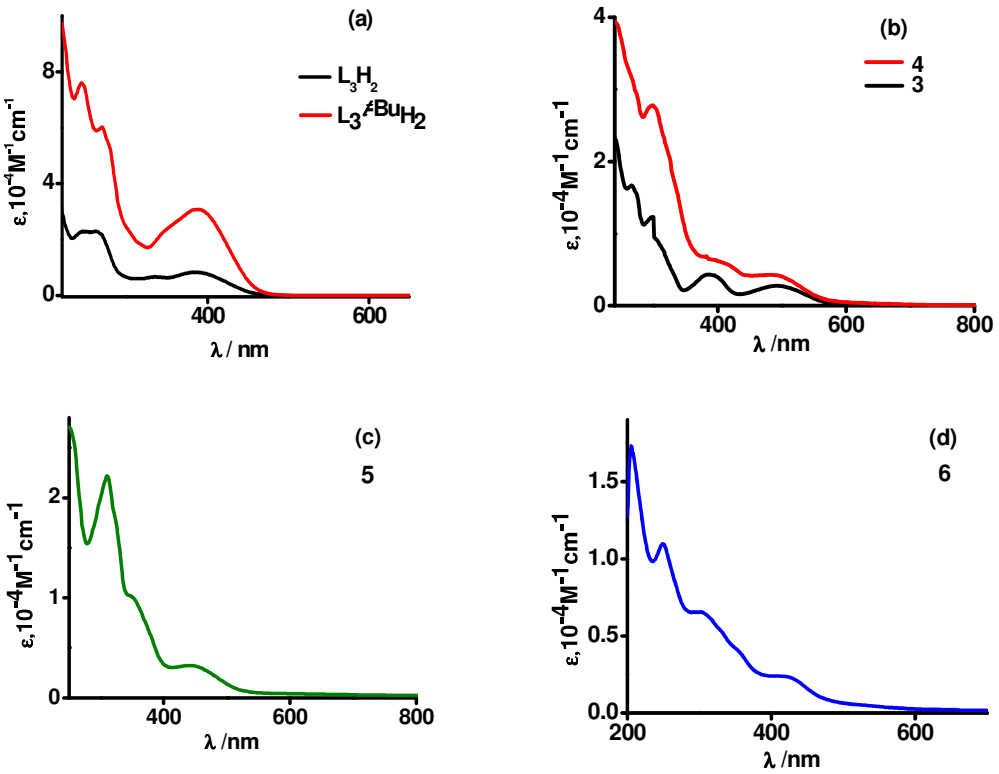


Fig. S1 UV-vis/NIR absorption spectra of (a) L_3H_2 (black) and $L_3{}^{t\text{-}Bu}H_2$ (red) (b) **3** (red) and **4** (black) (c) **5** and (d) **6** in CH_2Cl_2 at 298 K.

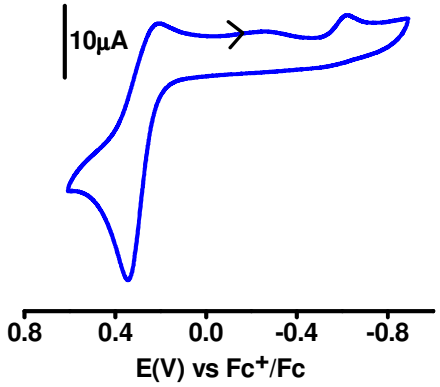


Fig. S2 Cyclic voltammogram of **3** in CH_2Cl_2 at 298 K. Conditions: 0.2 M $[N(n\text{-}Bu)_4]PF_6$ supporting electrolyte; scan rate 100 mVs^{-1}; platinum working electrode.

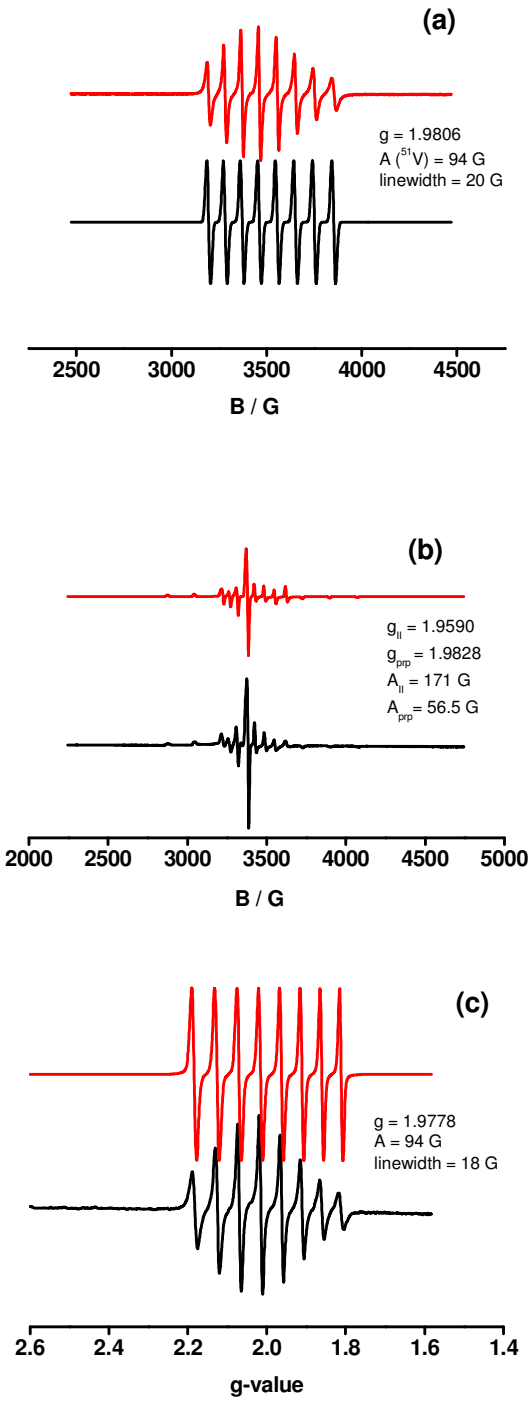


Fig. S3 X-band EPR spectra of (a) **3** in CH_2Cl_2 at 298 K (b) frozen CH_2Cl_2 glass of **3** at 25 K (c) **4** in CH_2Cl_2 at 298 K (black, experimental spectra; red, simulated spectra).

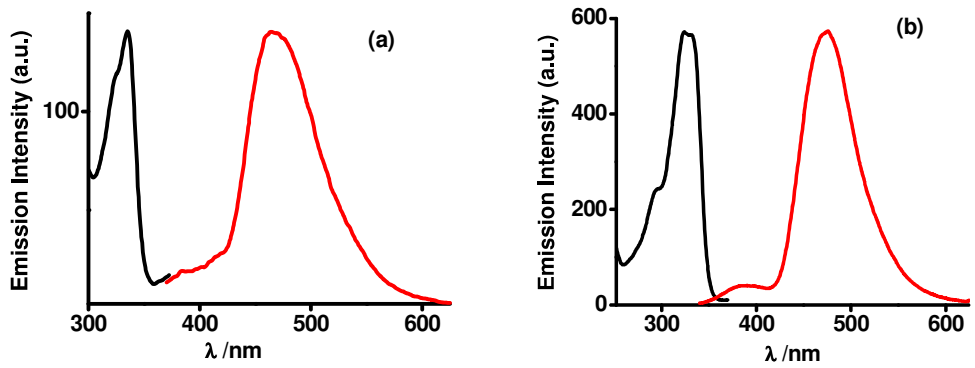
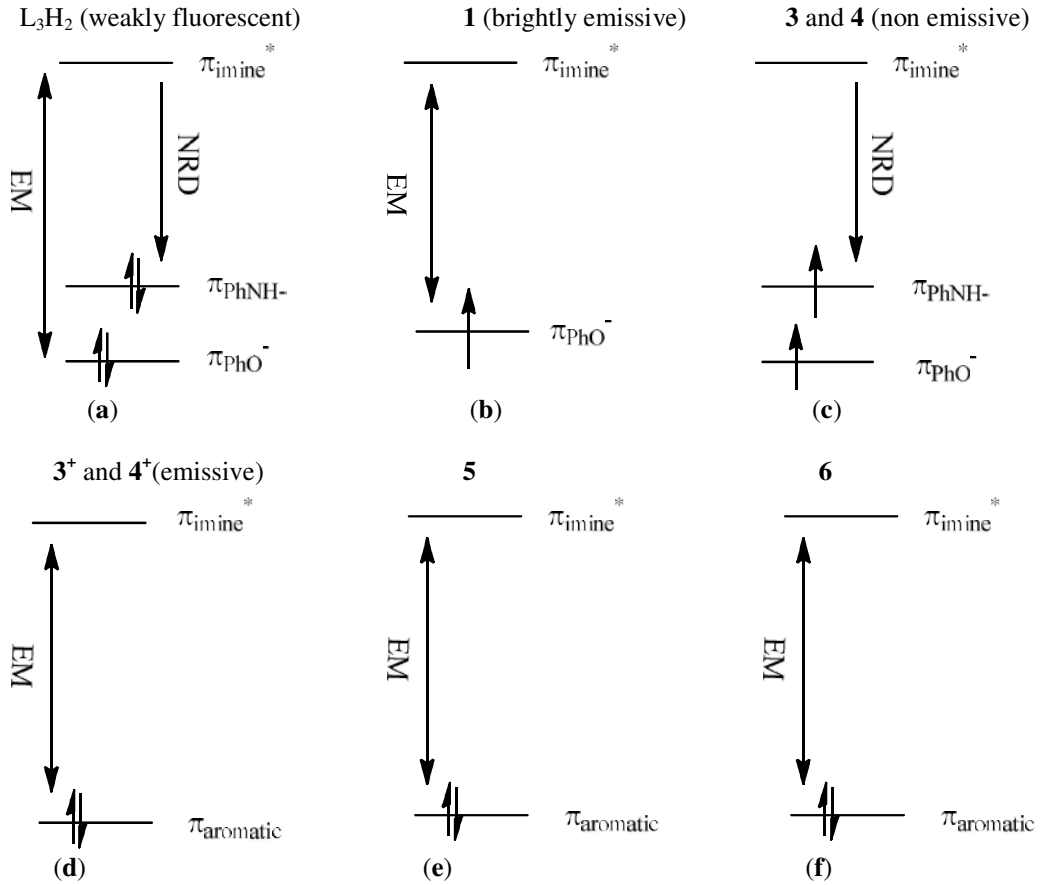


Fig. S4 Fluorescence spectra of (a) **5** and (b) **6** (black, excitation spectra; red, emission spectra) in CH_2Cl_2 at 298 K.

Scheme S1 Photoactive molecular orbitals (EM = Emission; NRD = Non-radiative decay)



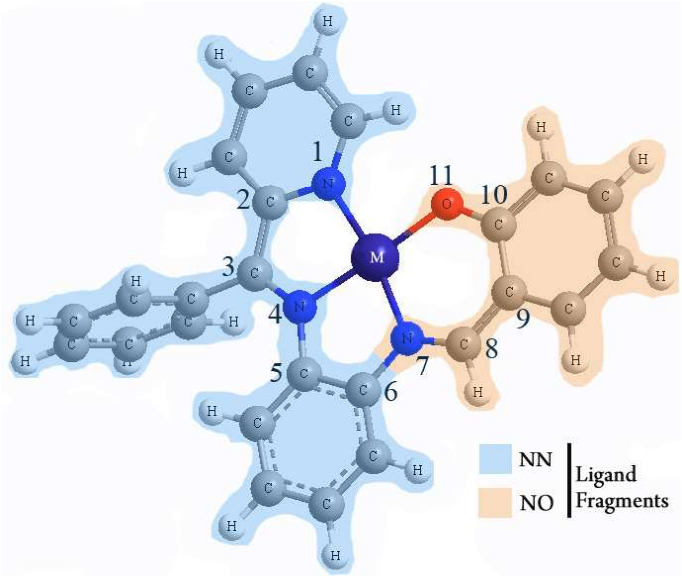


Fig. S5 Schematic diagram of the ligand fragmentation considered in MO analyses (Table S3).

Table S1 Calculated bond lengths (Å) of **3**, $\mathbf{3}^{+}$ and **6** (Fig. S5)

	3 (M = V)	**3^{+} (M = V)**	**6 (M = Co)**
M-N(7)	2.066	2.062	1.896
M-N(4)	1.968	1.919	1.916
M-N(1)	2.110	2.052	1.945
M-O(11)	1.923	1.794	1.888
N(4)-C(3)	1.448	1.465	1.299
C(3)-C(2)	1.530	1.513	1.476
C(2)-N(1)	1.348	1.349	1.355
N(16)-C(15)	1.381	1.393	1.406
C(5)-C(6)	1.428	1.416	1.423
C(6)-N(7)	1.414	1.407	1.404
N(7)-C(8)	1.302	1.305	1.306
C(8)-C(9)	1.435	1.437	1.420
C(9)-C(10)	1.435	1.423	1.443
C(10)-O(11)	1.316	1.350	1.293
M-O (Oxo)	1.599	1.580	-
M-Cl (Avg.)	-	-	2.306

Table S2 Excitation energies (λ/nm), oscillator strengths (f), transition types, and dominant contributions of UV−vis/NIR absorption bands of **6**, **3** and $\mathbf{3}^{+}$ obtained from TD DFT calculations

λ_{calc} / nm	f	λ_{exp}	Significant contributions (>10%)	Transition types	Dominant contributions
6					
591.5	0.0394		HOMO→LUMO (97%)	$\pi_{NO}(84)\rightarrow\pi_{NN}^{*}(92)$	LLCT
421.8	0.0891	423	HOMO-1→LUMO (10%) HOMO→LUMO+2 (54%)	$\pi_{NO}(14)+p_{Cl}(76)\rightarrow\pi_{NN}^{*}(92)$ $\pi_{NO}(84)\rightarrow\pi_{NN}^{*}(33)+\pi_{NO}^{*}(65)$	MLClLCT LLCT
412.2	0.0684		HOMO-15→LUMO+3 (28%) HOMO-10→LUMO+3 (11%) HOMO-1→LUMO (20%) HOMO→LUMO+2 (25%)	$d_{Co}(71)+\pi_{NO}(18)\rightarrow\pi_{NN}^{*}(99)$ $\pi_{NN}(85)+\pi_{NO}(11)\rightarrow\pi_{NN}^{*}(99)$ $\pi_{NO}(14)+p_{Cl}(76)\rightarrow\pi_{NN}^{*}(92)$ $\pi_{NO}(84)\rightarrow\pi_{NN}^{*}(33)+\pi_{NO}^{*}(65)$	MMLLCT LLCT MLClLCT LLCT
410.5	0.1537		HOMO-15→LUMO+3 (15%) HOMO-1→LUMO (59%)	$d_{Co}(71)+\pi_{NO}(18)\rightarrow\pi_{NN}^{*}(99)$ $\pi_{NO}(14)+p_{Cl}(76)\rightarrow\pi_{NN}^{*}(92)$	MMLLCT MLClLCT
396.4	0.0222		HOMO-15→LUMO+1 (21%) HOMO-10→LUMO+1 (24%)	$d_{Co}(71)+\pi_{NO}(18)\rightarrow d_{Co}(57)+p_{Cl}(33)$ $\pi_{NN}(85)+\pi_{NO}(11)\rightarrow d_{Co}(57)+p_{Cl}(33)$	d-d LMCT
360.9	0.0131		HOMO-5→LUMO (72%) HOMO-2→LUMO (11%)	$p_{Cl}(93)\rightarrow\pi_{NN}^{*}(92)$ $p_{Cl}(82)\rightarrow\pi_{NN}^{*}(92)$	ClLCT ClLCT
350.9	0.1472	352	HOMO-6→LUMO (15%) HOMO-5→LUMO (22%) HOMO-2→LUMO (42%)	$\pi_{NN}(85)+\pi_{NO}(12)\rightarrow\pi_{NN}^{*}(92)$ $p_{Cl}(93)\rightarrow\pi_{NN}^{*}(92)$ $p_{Cl}(82)\rightarrow\pi_{NN}^{*}(92)$	LLCT ClLCT ClLCT
344.7	0.0759		HOMO-8→LUMO+1 (20%) HOMO-6→LUMO (51%)	$d_{Co}(19)+\pi_{NN}(19)+\pi_{NO}(58)\rightarrow d_{Co}(57)+p_{Cl}(33)$ $\pi_{NN}(85)+\pi_{NO}(12)\rightarrow\pi_{NN}^{*}(92)$	MMLMCT LLCT
341.4	0.0563		HOMO-10→LUMO+1 (11%) HOMO-8→LUMO+1 (17%) HOMO-7→LUMO+1 (21%) HOMO→LUMO+4 (11%)	$\pi_{NN}(85)+\pi_{NO}(11)\rightarrow d_{Co}(57)+p_{Cl}(33)$ $d_{Co}(19)+\pi_{NN}(19)+\pi_{NO}(58)\rightarrow d_{Co}(57)+p_{Cl}(33)$ $d_{Co}(15)+p_{Cl}(71)\rightarrow d_{Co}(57)+p_{Cl}(33)$ $\pi_{NO}(84)\rightarrow d_{Co}(51)+\pi_{NN}^{*}(35)+\pi_{NO}^{*}(14)$	LMCT MMLMCT d-d LMMLCT
336.8	0.0603	331	HOMO→LUMO+4 (85%)	$\pi_{NO}(84)\rightarrow d_{Co}(51)+\pi_{NN}^{*}(35)+\pi_{NO}^{*}(14)$	LMMLCT
318.1	0.4507	303	HOMO-1→LUMO+2 (78%)	$\pi_{NO}(14)+p_{Cl}(76)\rightarrow\pi_{NN}^{*}(33)+\pi_{NO}^{*}(65)$	MLClLCT
3					
493.6	0.1329	496	αHOMO→LUMO (44%) βHOMO→LUMO (45%)	$\pi_{NN}(84)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(75)$ $\pi_{NN}(84)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(76)$	LLCT LLCT
427.9	0.0124		αHOMO-2→LUMO+8 (16%) βHOMO→LUMO+1 (43%)	$d_{VO}(73)+\pi_{NO}(18)\rightarrow d_{VO}(18)+\pi_{NN}^{*}(49)+\pi_{NO}^{*}(32)$ $\pi_{NN}(84)\rightarrow\pi_{NN}^{*}(92)$	MMLMMLCT LLCT
424.1	0.0241		αHOMO-2→LUMO+8 (23%) αHOMO→LUMO+1 (15%) βHOMO→LUMO+1 (20%)	$d_{VO}(73)+\pi_{NO}(18)\rightarrow d_{VO}(18)+\pi_{NN}^{*}(49)+\pi_{NO}^{*}(32)$ $\pi_{NN}(84)\rightarrow\pi_{NN}^{*}(90)$ $\pi_{NN}(84)\rightarrow\pi_{NN}^{*}(92)$	MMLMMLCT LLCT LLCT
380.5	0.0493	386	αHOMO-2→LUMO (12%) αHOMO-1→LUMO (20%) βHOMO-1→LUMO (20%)	$d_{VO}(73)+\pi_{NO}(18)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(75)$ $\pi_{NN}(14)+\pi_{NO}(77)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(75)$ $\pi_{NN}(17)+\pi_{NO}(81)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(76)$	MMLLCT LLCT LLCT
375.9	0.0804		αHOMO-2→LUMO (14%) αHOMO-1→LUMO (21%) βHOMO-1→LUMO (24%)	$d_{VO}(73)+\pi_{NO}(18)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(75)$ $\pi_{NN}(14)+\pi_{NO}(77)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(75)$ $\pi_{NN}(17)+\pi_{NO}(81)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(76)$	MMLLCT LLCT LLCT
366.1	0.0181		αHOMO→LUMO+2 (49%) αHOMO→LUMO+3 (32%)	$\pi_{NN}(84)\rightarrow\pi_{NN}^{*}(98)$ $\pi_{NN}(84)\rightarrow d_{VO}(65)+\pi_{NN}^{*}(30)$	LLCT LMMLCT
357.1	0.0114		αHOMO→LUMO+3 (19%) αHOMO→LUMO+5 (13%) βHOMO→LUMO+3 (13%)	$\pi_{NN}(84)\rightarrow d_{VO}(65)+\pi_{NN}^{*}(30)$ $\pi_{NN}(84)\rightarrow d_{VO}(19)+\pi_{NN}^{*}(77)$ $\pi_{NN}(84)\rightarrow d_{VO}(75)+\pi_{NN}^{*}(19)$	LMMLCT LMMLCT LMMLCT
337.1	0.0121	327	αHOMO→LUMO+2 (16%) αHOMO→LUMO+4 (25%) βHOMO→LUMO+3 (20%)	$\pi_{NN}(84)\rightarrow\pi_{NN}^{*}(98)$ $\pi_{NN}(84)\rightarrow d_{VO}(10)+\pi_{NN}^{*}(89)$ $\pi_{NN}(84)\rightarrow d_{VO}(75)+\pi_{NN}^{*}(19)$	LLCT LMMLCT LMMLCT
316.7	0.1876	313	αHOMO-3→LUMO (39%) βHOMO-2→LUMO (42%)	$\pi_{NN}(50)+\pi_{NO}(49)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(75)$ $\pi_{NN}(51)+\pi_{NO}(48)\rightarrow\pi_{NN}^{*}(18)+\pi_{NO}^{*}(76)$	LLCT LLCT
308.8	0.0204	300	βHOMO-1→LUMO+2 (55%)	$\pi_{NN}(17)+\pi_{NO}(81)\rightarrow\pi_{NN}^{*}(93)$	LLCT
$\mathbf{3}^{+}$					
640.9	0.0119		HOMO-4→LUMO (11%) HOMO-2→LUMO (83%)	$\pi_{NN}(21)+\pi_{NO}(77)\rightarrow d_{VO}(80)+\pi_{NO}^{*}(13)$ $\pi_{NN}(97)\rightarrow d_{VO}(80)+\pi_{NO}^{*}(13)$	LMMLCT LMMLCT
471.5	0.0764	491	HOMO→LUMO+2 (80%)	$\pi_{NN}(80)+\pi_{NO}(12)\rightarrow d_{VO}(10)+\pi_{NN}^{*}(26)+\pi_{NO}^{*}(64)$	LMMLCT

λ_{calc} / nm	f	λ_{exp}	Significant Contributions (>10%)	Transition Types	Dominant Contributions
439.7	0.0308		HOMO-1→LUMO+1 (85%)	$\pi_{NN}(58)+\pi_{NO}(41)\rightarrow d_{VO}(71)+\pi_{NN}^{*}(15)+\pi_{NO}^{*}(14)$	LMMLCT
391.4	0.0140	407	HOMO→LUMO+3 (39%) HOMO→LUMO+5 (39%)	$\pi_{NN}(80)+\pi_{NO}(12)\rightarrow d_{VO}(26)+\pi_{NN}^{*}(67)$ $\pi_{NN}(80)+\pi_{NO}(12)\rightarrow d_{VO}(50)+\pi_{NN}^{*}(35)+\pi_{NO}^{*}(15)$	LMMLCT LMMLCT
377.2	0.0132	376	HOMO-4→LUMO+1 (35%) HOMO-3→LUMO+1 (12%) HOMO→LUMO+3 (22%) HOMO→LUMO+5 (23%)	$\pi_{NN}(21)+\pi_{NO}(77)\rightarrow d_{VO}(71)+\pi_{NN}^{*}(15)+\pi_{NO}^{*}(14)$ $\pi_{NO}(98)\rightarrow d_{VO}(71)+\pi_{NN}^{*}(15)+\pi_{NO}^{*}(14)$ $\pi_{NN}(80)+\pi_{NO}(12)\rightarrow d_{VO}(26)+\pi_{NN}^{*}(67)$ $\pi_{NN}(80)+\pi_{NO}(12)\rightarrow d_{VO}(50)+\pi_{NN}^{*}(35)+\pi_{NO}^{*}(15)$	LMMLCT LMMLCT LMMLCT LMMLCT
363.2	0.0122		HOMO-7→LUMO (80%)	$\pi_{NN}(93)\rightarrow d_{VO}(80)+\pi_{NO}^{*}(13)$	LMMLCT
357.8	0.1182		HOMO-1→LUMO+2 (61%)	$\pi_{NN}(58)+\pi_{NO}(41)\rightarrow d_{VO}(10)+\pi_{NN}^{*}(26)+\pi_{NO}^{*}(64)$	LMMLCT
342.5	0.0119		HOMO-2→LUMO+2 (95%)	$\pi_{NN}(97)\rightarrow d_{VO}(10)+\pi_{NN}^{*}(26)+\pi_{NO}^{*}(64)$	LMMLCT
326.5	0.0167	331	HOMO-4→LUMO+2 (12%) HOMO→LUMO+6 (70%)	$\pi_{NN}(21)+\pi_{NO}(77)\rightarrow d_{VO}(10)+\pi_{NN}^{*}(26)+\pi_{NO}^{*}(64)$ $\pi_{NN}(80)+\pi_{NO}(12)\rightarrow \pi_{NN}^{*}(93)$	LMMLCT LLCT
324.7	0.0288		HOMO-10→LUMO (36%) HOMO-4→LUMO+2 (11%) HOMO-1→LUMO+5 (11%) HOMO→LUMO+6 (19%)	$d_{VO}(15)+\pi_{NN}(32)+\pi_{NO}(53)\rightarrow d_{VO}(80)+\pi_{NO}^{*}(13)$ $\pi_{NN}(21)+\pi_{NO}(77)\rightarrow d_{VO}(10)+\pi_{NN}^{*}(26)+\pi_{NO}^{*}(64)$ $\pi_{NN}(58)+\pi_{NO}(41)\rightarrow d_{VO}(50)+\pi_{NN}^{*}(35)+\pi_{NO}^{*}(15)$ $\pi_{NN}(80)+\pi_{NO}(12)\rightarrow \pi_{NN}^{*}(93)$	MMLMMLCT LMMLCT LMMLCT LLCT
321.9	0.0182		HOMO-10→LUMO (26%) HOMO-4→LUMO+2 (56%)	$d_{VO}(15)+\pi_{NN}(32)+\pi_{NO}(53)\rightarrow d_{VO}(80)+\pi_{NO}^{*}(13)$ $\pi_{NN}(21)+\pi_{NO}(77)\rightarrow d_{VO}(10)+\pi_{NN}^{*}(26)+\pi_{NO}^{*}(64)$	MMLMMLCT LMMLCT
307.2	0.0332		HOMO→LUMO+7 (64%)	$\pi_{NN}(80)+\pi_{NO}(12)\rightarrow d_{VO}(68)+\pi_{NN}^{*}(20)+\pi_{NO}^{*}(13)$	LMMLCT
303.4	0.0321		HOMO-5→LUMO+1 (55%) HOMO-1→LUMO+3 (23%)	$\pi_{NN}(31)+\pi_{NO}(69)\rightarrow d_{VO}(71)+\pi_{NN}^{*}(15)+\pi_{NO}^{*}(14)$ $\pi_{NN}(58)+\pi_{NO}(41)\rightarrow d_{VO}(26)+\pi_{NN}^{*}(67)$	LMMLCT LMMLCT
303.3	0.0434		HOMO-5→LUMO+1 (26%) HOMO-1→LUMO+3 (53%)	$\pi_{NN}(31)+\pi_{NO}(69)\rightarrow d_{VO}(71)+\pi_{NN}^{*}(15)+\pi_{NO}^{*}(14)$ $\pi_{NN}(58)+\pi_{NO}(41)\rightarrow d_{VO}(26)+\pi_{NN}^{*}(67)$	LMMLCT LMMLCT
300.7	0.0116		HOMO-2→LUMO+3 (95%)	$\pi_{NN}(97)\rightarrow d_{VO}(26)+\pi_{NN}^{*}(67)$	LMMLCT

LLCT = Ligand to Ligand Charge Transfer, MLClLCT = Mixed Ligand Chloride to Ligand Charge Transfer, MMLLCT = Mixed Metal Ligand to Ligand Charge Transfer, d-d = d-d Transition, ClLCT = Chloride to Ligand Charge Transfer, MMLMCT = Mixed Metal Ligand to Metal Charge Transfer, LMCT = Ligand to Metal Charge Transfer, LMMLCT = Ligand to Mixed Metal Ligand Charge Transfer, MMLMMLCT = Mixed Metal Ligand to Mixed Metal Ligand Charge Transfer

Table S3 Population analyses of selected molecular orbitals of **6**, **3** and $\mathbf{3}^{+}$

	6			**3**						$\mathbf{3}^{+}$		
MO	Co	NN	NO	VO		NN		NO		VO	NN	NO
				α	β	α	β	α	β			
LUMO	1	92	6	7	5	18	18	75	76	80	7	13
HOMO	2	9	84	7	6	84	84	9	9	8	80	12
HOMO-1	4	6	14	9	3	14	17	77	81	2	58	41
HOMO-2	8	3	6	73	1	9	51	18	48	0	97	2
HOMO-3	8	27	44	1	0	50	95	49	5	0	98	2
HOMO-4	6	2	0	1	0	94	100	5	0	3	21	77
HOMO-5	2	7	0	0	2	100	39	0	60	0	31	69
HOMO-6	2	85	12	2	28	40	26	59	47	2	93	5
HOMO-7	15	8	6	33	4	49	67	18	29	5	93	1
HOMO-8	19	19	58	12	15	55	76	33	10	6	80	15
HOMO-9	1	60	39	12	69	68	21	20	10	9	88	3
HOMO-10	4	85	11	66	24	22	69	11	7	15	32	53
HOMO-11	1	89	10	22	45	67	22	10	33	4	95	1
HOMO-12	38	36	23	41	34	19	47	40	19	11	51	38
HOMO-13	52	36	8	19	37	58	41	22	22	3	77	20
HOMO-14	14	75	9	43	26	38	67	19	7	5	47	48
HOMO-15	71	9	18	29	22	63	17	8	61	4	83	13

Table S4 Optimized coordinates of **3**

Sl	Symbol	X	Y	Z	Sl	Symbol	X	Y	Z
1	O	8.147164	4.124388	13.00194	26	C	8.690336	-0.98481	8.874736
2	C	8.001572	5.392101	12.67864	27	C	8.382123	-2.3409	8.731882
3	C	8.927784	6.337502	13.18016	28	C	7.564312	-2.96576	9.673843
4	C	8.840584	7.677888	12.84445	29	C	7.060919	-2.23614	10.75415
5	C	7.831554	8.143669	11.97977	30	H	9.709048	5.970464	13.83879
6	C	6.921945	7.239967	11.46586	31	H	9.565588	8.378326	13.25191
7	C	6.968513	5.864152	11.80179	32	H	7.772338	9.195693	11.7187
8	C	6.017899	4.985596	11.18224	33	H	6.139927	7.579367	10.78948
9	N	5.857557	3.725785	11.4709	34	H	5.412726	5.422217	10.38315
10	C	4.994388	2.848151	10.77434	35	H	3.67663	4.276108	9.836635
11	C	3.925232	3.225618	9.959822	36	H	2.309608	2.546198	8.708082
12	C	3.148761	2.252716	9.331441	37	H	2.843923	0.13838	9.042958
13	C	3.449106	0.90057	9.527371	38	H	4.719707	-0.54766	10.47673
14	C	4.507753	0.50689	10.34381	39	H	6.056212	-0.7039	12.58734
15	C	5.306569	1.471796	10.98915	40	H	8.531657	-2.03277	13.21985
16	N	6.382484	1.243532	11.82372	41	H	10.32311	-1.6574	14.91716
17	C	6.852454	-0.09347	12.12015	42	H	10.75617	0.682757	15.73134
18	C	7.97028	0.042354	13.15611	43	H	9.323059	2.539271	14.81264
19	C	8.725441	-1.04091	13.61313	44	H	8.417147	0.797796	10.06053
20	C	9.729961	-0.82401	14.55132	45	H	9.320803	-0.49063	8.140141
21	C	9.974987	0.473852	15.00829	46	H	8.771357	-2.90353	7.887611
22	C	9.189207	1.504997	14.51346	47	H	7.309553	-4.01685	9.565952
23	N	8.207974	1.285723	13.61887	48	H	6.409885	-2.72341	11.47812
24	C	7.370769	-0.87988	10.90681	49	V	6.80704	2.745641	13.0217
25	C	8.189391	-0.2592	9.954997	50	O	5.82714	2.861401	14.27981

Table S5 Optimized coordinates of $\mathbf{3}^{+}$

Sl	Symbol	X	Y	Z	Sl	Symbol	X	Y	Z
1	O	8.259827	4.00035	12.52	10	C	4.969604	2.811675	10.78159
2	C	8.11713	5.337422	12.39937	11	C	3.892789	3.164095	9.961542
3	C	9.123176	6.198078	12.84363	12	C	3.083213	2.16284	9.436345
4	C	8.974466	7.570627	12.66625	13	C	3.35792	0.817781	9.720863
5	C	7.838842	8.098245	12.03035	14	C	4.433123	0.456507	10.52748
6	C	6.850025	7.244578	11.57044	15	C	5.261989	1.455194	11.06607
7	C	6.956597	5.846451	11.75256	16	N	6.396953	1.25777	11.84922
8	C	5.943197	4.980592	11.21542	17	C	6.889146	-0.09956	12.09521
9	N	5.879513	3.689897	11.39748	18	C	7.937971	0.011369	13.18002

Sl	Symbol	X	Y	Z	Sl	Symbol	X	Y	Z
19	C	8.66092	-1.06782	13.68733	35	H	3.670644	4.204619	9.747028
20	C	9.569891	-0.85043	14.7179	36	H	2.235629	2.426274	8.812431
21	C	9.750153	0.44409	15.21965	37	H	2.72315	0.040596	9.306242
22	C	9.013175	1.477267	14.66723	38	H	4.633806	-0.59028	10.71859
23	N	8.129022	1.255383	13.66627	39	H	6.071935	-0.71712	12.50369
24	C	7.439492	-0.81343	10.85902	40	H	8.508723	-2.05628	13.26846
25	C	8.321345	-0.16153	9.987753	41	H	10.13543	-1.68066	15.12968
26	C	8.849038	-0.8387	8.889094	42	H	10.45046	0.648703	16.02164
27	C	8.506445	-2.17364	8.654384	43	H	9.112388	2.502416	15.00751
28	C	7.629311	-2.82847	9.519823	44	H	8.583981	0.878824	10.16146
29	C	7.095949	-2.14889	10.61749	45	H	9.527711	-0.32493	8.214409
30	H	10.00521	5.78064	13.31746	46	H	8.917723	-2.69814	7.797026
31	H	9.754018	8.238954	13.0193	47	H	7.352144	-3.8628	9.338653
32	H	7.740107	9.169936	11.89431	48	H	6.401922	-2.66	11.28244
33	H	5.973968	7.643006	11.06578	49	V	7.000071	2.77012	12.86396
34	H	5.186177	5.452797	10.58827	50	O	6.024254	3.215215	14.02371

Table S6 Optimized coordinates of **6**

Sl	Symbol	X	Y	Z	Sl	Symbol	X	Y	Z
1	C	0.954017	1.826494	8.8E-06	21	C	-4.77126	-1.41164	-2.1E-05
2	C	-0.36361	2.363533	9.1E-06	22	C	-6.02764	-0.843	-2.5E-05
3	C	-0.5299	3.757791	2.3E-06	23	H	-7.1957	0.996462	-2.1E-05
4	C	0.5782	4.598736	-5E-06	24	H	-4.6401	-2.4895	-2.7E-05
5	C	1.874776	4.068228	-6.3E-06	25	H	-6.90288	-1.48913	-3.5E-05
6	C	2.06265	2.690243	8E-07	26	C	1.557309	-1.84149	1.5E-06
7	H	-1.52207	4.19447	2.6E-06	27	C	2.436875	-2.92727	-5.8E-06
8	H	0.430659	5.675297	-1E-05	28	C	1.907916	-4.21995	-9.7E-06
9	H	2.737283	4.72818	-1.3E-05	29	H	3.507774	-2.75948	-8.5E-06
10	H	3.066304	2.290482	3E-07	30	C	-0.29729	-3.26221	2.8E-06
11	N	-1.40961	1.427555	1.33E-05	31	C	0.524759	-4.39314	-5.2E-06
12	N	0.990136	0.421301	1.54E-05	32	H	2.572354	-5.07935	-1.6E-05
13	C	-2.67817	1.737325	0.000008	33	H	-1.38091	-3.31211	6.4E-06
14	H	-2.95269	2.792599	9.6E-06	34	H	0.078633	-5.38227	-8.1E-06
15	C	1.974981	-0.42567	5.7E-06	35	N	0.216418	-2.03493	6.4E-06
16	C	-3.76401	0.82164	-8E-07	36	O	-2.44446	-1.21239	-5.3E-06
17	C	-5.08126	1.365611	-5.1E-06	37	Co	-0.76226	-0.35436	9.8E-06
18	C	-3.58912	-0.61065	-9.6E-06	38	Cl	-0.70852	-0.35153	2.305328
19	C	-6.20017	0.563317	-1.7E-05	39	Cl	-0.70849	-0.35149	-2.30531
20	H	-5.18948	2.448848	1.2E-06	40	C	3.432489	-0.10461	4E-07

Sl	Symbol	X	Y	Z	Sl	Symbol	X	Y	Z
41	C	4.124387	0.019604	1.214351	46	H	3.586632	-0.08212	-2.15361
42	C	4.124385	0.019568	-1.21436	47	C	6.183424	0.418591	-9.4E-06
43	C	5.496522	0.284172	1.210959	48	H	6.026861	0.384698	2.154162
44	H	3.586635	-0.08206	2.153607	49	H	6.026858	0.384635	-2.15418
45	C	5.496521	0.284136	-1.21097	50	H	7.250445	0.624964	-1.3E-05

END