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Formation of metal-radical species upon reduction of cobalt(II), nickel(II) and copper(II) complexes with heteroleptic ligands: experimental and theoretical study

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Table S1 Experimental (X-ray) bond lengths of complex **1**

Atoms		Length/Å	Atoms		Length/Å
Se1	N3	1.807(4)	C5	C6	1.338(7)
Se1	N4	1.796(5)	C6	C10	1.414(8)
Se2	N6	1.793(4)	C7	C8	1.404(8)
Se2	N7	1.781(5)	C7	C10	1.481(7)
Co1	O1	2.019(4)	C8	C1A	1.501(2)
Co1	O3	2.111(3)	C8	C1B	1.501(2)
Co1	O4	2.034(4)	C9	C10	1.378(7)
Co1	O6	2.091(3)	C11	C12	1.452(8)
Co1	N1	2.103(4)	C13	C20	1.533(8)
Co1	N2	2.111(4)	C14	C20	1.362(7)
O1	C1A	1.250(2)	C15	C16	1.414(8)
O1	C1B	1.250(2)	C15	C21	1.486(7)
O3	C7	1.273(7)	C16	C17	1.409(7)
O4	C13	1.251(7)	C17	C18	1.335(7)
O5	C13	1.243(7)	C18	C22	1.438(8)
O6	C19	1.260(6)	C19	C20	1.407(7)
N1	C25	1.331(6)	C19	C22	1.476(7)
N1	C34	1.369(6)	C21	C22	1.394(7)
N2	C32	1.312(6)	C23	C24	1.512(7)
N2	C36	1.378(6)	C25	C26	1.378(7)
N3	C3	1.332(6)	C26	C27	1.355(8)
N4	C4	1.346(6)	C27	C33	1.410(7)
N5	C2	1.366(7)	C28	C29	1.342(8)
N5	C9	1.351(7)	C28	C33	1.432(8)
N5	C11	1.476(8)	C29	C35	1.442(7)
N6	C15	1.328(6)	C30	C31	1.368(7)
N7	C16	1.360(7)	C30	C35	1.410(7)
N8	C14	1.359(6)	C31	C32	1.388(7)
N8	C21	1.356(6)	C33	C34	1.386(7)
N8	C23	1.489(6)	C34	C36	1.437(7)
C2	C8	1.347(8)	C35	C36	1.386(7)
C3	C4	1.429(7)	O2A	C1A	1.40(2)
C3	C9	1.485(7)	O2B	C1B	1.24(4)
C4	C5	1.432(8)			

Table S2 Experimental (X-ray) bond angles of complex **1**

Atoms			Angle/°	Atoms			Angle/°
N4	Se1	N3	94.4(2)	C10	C9	C3	116.3(5)
N7	Se2	N6	94.6(2)	C6	C10	C7	116.8(5)
O1	Co1	O3	86.2(2)	C9	C10	C6	122.7(5)
O1	Co1	O4	178.9(2)	C9	C10	C7	120.5(5)
O1	Co1	O6	94.9(2)	C12	C11	N5	109.1(5)
O1	Co1	N1	89.3(2)	O4	C13	C20	117.4(6)
O1	Co1	N2	87.1(2)	O5	C13	O4	125.4(5)
O3	Co1	N2	173.0(2)	O5	C13	C20	117.1(5)
O4	Co1	O3	94.1(2)	N8	C14	C20	125.2(5)
O4	Co1	O6	86.2(2)	N6	C15	C16	117.9(5)
O4	Co1	N1	89.6(2)	N6	C15	C21	123.4(5)
O4	Co1	N2	92.5(2)	C16	C15	C21	118.6(5)
O6	Co1	O3	86.5(2)	N7	C16	C15	115.7(5)
O6	Co1	N1	173.7(2)	N7	C16	C17	121.7(5)
O6	Co1	N2	96.4(2)	C17	C16	C15	122.5(5)
N1	Co1	O3	98.6(2)	C18	C17	C16	118.6(5)
N1	Co1	N2	79.1(2)	C17	C18	C22	122.2(5)
C1A	O1	Co1	129.7(6)	O6	C19	C20	125.1(5)
C1B	O1	Co1	128(2)	O6	C19	C22	119.1(5)
C7	O3	Co1	118.9(3)	C20	C19	C22	115.8(5)
C13	O4	Co1	130.1(4)	C14	C20	C13	118.2(5)
C19	O6	Co1	117.5(3)	C14	C20	C19	119.3(5)
C25	N1	Co1	129.5(4)	C19	C20	C13	122.4(5)
C25	N1	C34	117.0(4)	N8	C21	C15	122.8(4)
C34	N1	Co1	113.5(3)	N8	C21	C22	121.2(5)
C32	N2	Co1	129.3(3)	C22	C21	C15	116.0(5)
C32	N2	C36	117.8(4)	C18	C22	C19	118.0(5)
C36	N2	Co1	112.7(3)	C21	C22	C18	121.9(5)
C3	N3	Se1	105.8(4)	C21	C22	C19	120.0(5)
C4	N4	Se1	105.8(4)	N8	C23	C24	112.7(4)
C2	N5	C11	115.7(5)	N1	C25	C26	123.6(5)
C9	N5	C2	117.7(5)	C27	C26	C25	119.1(5)
C9	N5	C11	126.6(4)	C26	C27	C33	120.0(5)
C15	N6	Se2	105.7(4)	C29	C28	C33	122.5(5)
C16	N7	Se2	106.0(4)	C28	C29	C35	120.3(5)
C14	N8	C23	116.9(5)	C31	C30	C35	119.2(5)
C21	N8	C14	118.1(4)	C30	C31	C32	119.0(5)
C21	N8	C23	124.9(4)	N2	C32	C31	123.9(5)
C8	C2	N5	126.5(6)	C27	C33	C28	125.0(5)
N3	C3	C4	117.2(4)	C34	C33	C27	117.0(5)
N3	C3	C9	124.2(5)	C34	C33	C28	117.9(5)
C4	C3	C9	118.5(5)	N1	C34	C33	123.0(4)
N4	C4	C3	116.7(5)	N1	C34	C36	116.9(4)
N4	C4	C5	121.9(5)	C33	C34	C36	120.1(5)
C3	C4	C5	121.4(5)	C30	C35	C29	123.7(5)
C6	C5	C4	118.0(5)	C36	C35	C29	118.3(5)
C5	C6	C10	122.9(5)	C36	C35	C30	118.0(4)
O3	C7	C8	125.5(5)	N2	C36	C34	117.1(4)
O3	C7	C10	118.4(5)	N2	C36	C35	122.2(4)
C8	C7	C10	116.1(5)	C35	C36	C34	120.7(4)
C2	C8	C7	118.0(5)	O1	C1A	C8	119.2(5)
C2	C8	C1A	116.8(6)	O1	C1A	O2A	122(2)
C2	C8	C1B	116.3(6)	O2A	C1A	C8	114(2)
C7	C8	C1A	125.2(6)	O1	C1B	C8	119.2(5)
C7	C8	C1B	125.7(6)	O2B	C1B	O1	116(3)
N5	C9	C3	122.9(5)	O2B	C1B	C8	115(2)
N5	C9	C10	120.8(5)				

Table S3 Experimental (X-ray) bond lengths of complex **2**

Atoms		Length/Å	Atoms		Length/Å
Se1	N3	1.795(3)	C5	C6	1.341(5)
Se1	N4	1.782(4)	C6	C10	1.436(5)
Se2	N6	1.778(3)	C7	C8	1.424(5)
Se2	N7	1.782(4)	C7	C10	1.447(5)
Ni1	O1	1.999(3)	C8	C1A	1.48(3)
Ni1	O3	2.073(3)	C8	C1B	1.56(2)
Ni1	O4	2.037(3)	C9	C10	1.406(5)
Ni1	O6	2.066(2)	C11	C12	1.460(7)
Ni1	N1	2.068(3)	C13	C20	1.502(5)
Ni1	N2	2.074(3)	C14	C20	1.347(5)
O1	C1A	1.41(3)	C15	C16	1.443(5)
O1	C1B	1.15(2)	C15	C21	1.452(5)
O3	C7	1.274(4)	C16	C17	1.420(5)
O4	C13	1.255(5)	C17	C18	1.347(5)
O5	C13	1.246(5)	C18	C22	1.431(5)
O6	C19	1.265(4)	C19	C20	1.433(5)
N1	C25	1.314(5)	C19	C22	1.446(5)
N1	C34	1.353(5)	C21	C22	1.394(5)
N2	C32	1.323(5)	C23	C24	1.501(6)
N2	C36	1.362(4)	C25	C26	1.393(6)
N3	C3	1.335(5)	C26	C27	1.363(7)
N4	C4	1.328(5)	C27	C33	1.402(6)
N5	C2	1.335(5)	C28	C29	1.344(6)
N5	C9	1.365(5)	C28	C33	1.430(6)
N5	C11	1.484(5)	C29	C35	1.436(5)
N6	C15	1.329(5)	C30	C31	1.363(6)
N7	C16	1.328(5)	C30	C35	1.382(6)
N8	C14	1.352(5)	C31	C32	1.383(6)
N8	C21	1.383(5)	C33	C34	1.404(5)
N8	C23	1.500(4)	C34	C36	1.430(5)
C2	C8	1.355(5)	C35	C36	1.397(5)
C3	C4	1.438(5)	O2A	C1A	1.33(2)
C3	C9	1.463(5)	O2B	C1B	1.33(1)
C4	C5	1.433(6)			

Table S4 Experimental (X-ray) bond angles of complex **2**

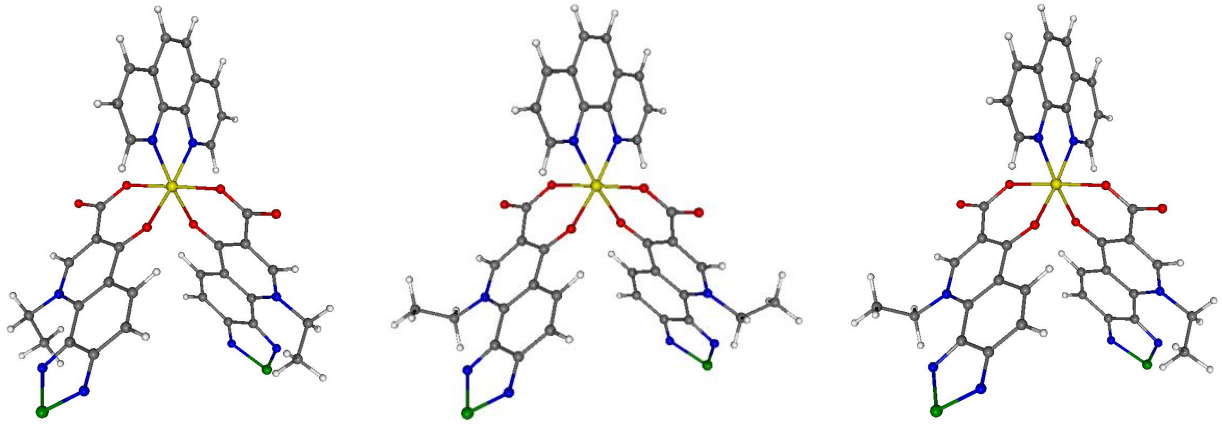
Atoms			Angle/°	Atoms			Angle/°
N4	Se1	N3	93.8(2)	C10	C9	C3	117.1(3)
N6	Se2	N7	94.1(2)	C6	C10	C7	118.0(3)
O1	Ni1	O3	88.1(1)	C9	C10	C6	120.8(3)
O1	Ni1	O4	178.5(1)	C9	C10	C7	121.2(3)
O1	Ni1	O6	93.5(1)	C12	C11	N5	110.5(4)
O1	Ni1	N1	88.9(1)	O4	C13	C20	119.5(4)
O1	Ni1	N2	86.9(1)	O5	C13	O4	122.8(4)
O3	Ni1	N2	174.2(1)	O5	C13	C20	117.7(4)
O4	Ni1	O3	93.2(1)	C20	C14	N8	125.6(4)
O4	Ni1	O6	87.4(1)	N6	C15	C16	116.1(3)
O4	Ni1	N1	90.1(1)	N6	C15	C21	124.9(3)
O4	Ni1	N2	91.8(1)	C16	C15	C21	118.9(3)
O6	Ni1	O3	86.9(1)	N7	C16	C15	115.8(4)
O6	Ni1	N1	175.7(1)	N7	C16	C17	123.4(4)
O6	Ni1	N2	96.3(1)	C17	C16	C15	120.8(3)
N1	Ni1	O3	96.7(1)	C18	C17	C16	118.5(4)
N1	Ni1	N2	80.3(2)	C17	C18	C22	123.1(3)
C1A	O1	Ni1	131.3(1)	O6	C19	C20	124.5(3)
C1B	O1	Ni1	128.9(5)	O6	C19	C22	120.1(3)
C7	O3	Ni1	119.6(2)	C20	C19	C22	115.4(3)
C13	O4	Ni1	128.5(2)	C14	C20	C13	118.1(4)
C19	O6	Ni1	118.1(2)	C14	C20	C19	119.1(3)
C25	N1	Ni1	129.1(3)	C19	C20	C13	122.8(3)
C25	N1	C34	118.4(3)	N8	C21	C15	122.9(3)
C34	N1	Ni1	112.4(2)	N8	C21	C22	119.0(3)
C32	N2	Ni1	130.0(3)	C22	C21	C15	118.0(3)
C32	N2	C36	117.3(3)	C18	C22	C19	117.5(3)
C36	N2	Ni1	112.2(2)	C21	C22	C18	120.4(3)
C3	N3	Se1	106.6(3)	C21	C22	C19	122.0(3)
C4	N4	Se1	107.2(3)	C24	C23	N8	112.4(3)
C2	N5	C9	118.8(3)	N1	C25	C26	122.7(4)
C2	N5	C11	115.4(3)	C27	C26	C25	119.5(4)
C9	N5	C11	125.8(3)	C26	C27	C33	119.5(4)
C15	N6	Se2	107.0(3)	C29	C28	C33	121.4(4)
C16	N7	Se2	107.1(3)	C28	C29	C35	121.5(4)
C14	N8	C21	118.7(3)	C31	C30	C35	119.7(4)
C14	N8	C23	116.7(3)	C30	C31	C32	119.0(4)
C21	N8	C23	124.6(3)	N2	C32	C31	123.5(4)
N5	C2	C8	126.5(4)	C27	C33	C28	124.3(4)
N3	C3	C4	116.1(3)	C27	C33	C34	117.0(4)
N3	C3	C9	124.7(4)	C34	C33	C28	118.6(4)
C4	C3	C9	119.2(3)	N1	C34	C33	122.7(4)
N4	C4	C3	116.3(4)	N1	C34	C36	117.6(3)
N4	C4	C5	122.6(4)	C33	C34	C36	119.7(3)
C5	C4	C3	121.1(3)	C30	C35	C29	124.0(4)
C6	C5	C4	118.1(4)	C30	C35	C36	117.9(4)
C5	C6	C10	123.3(4)	C36	C35	C29	118.1(4)
O3	C7	C8	124.6(3)	N2	C36	C34	116.8(3)
O3	C7	C10	119.4(3)	N2	C36	C35	122.5(4)
C8	C7	C10	116.0(3)	C35	C36	C34	120.7(3)
C2	C8	C7	118.0(3)	O1	C1A	C8	111(2)
C2	C8	C1A	113(1)	O2A	C1A	O1	111(2)
C2	C8	C1B	120.4(6)	O2A	C1A	C8	121(2)
C7	C8	C1A	129(1)	O1	C1B	C8	123.4(8)
C7	C8	C1B	121.6(6)	O1	C1B	O2B	126(1)
N5	C9	C3	123.7(3)	O2B	C1B	C8	109(2)
N5	C9	C10	119.2(3)				

Table S5 Experimental (X-ray) bond lengths of comlex **3**

Atoms		**Length/ Å**	**Atoms**		**Length/ Å**
Se1	N3	1.784(3)	C3	C4	1.443(5)
Se1	N4	1.787(3)	C3	C9	1.457(5)
Cu1	Cl1	2.576(2)	C4	C5	1.417(5)
Cu1	O1	1.924(3)	C5	C6	1.339(5)
Cu1	O3	1.928(3)	C6	C10	1.442(5)
Cu1	N1	2.014(3)	C7	C8	1.407(5)
Cu1	N2	2.007(3)	C7	C10	1.448(5)
O1	C1	1.271(5)	C9	C10	1.386(5)
O2	C1	1.238(5)	C11	C12	1.508(6)
O3	C7	1.276(5)	C13	C14	1.404(6)
N1	C13	1.322(5)	C14	C15	1.385(7)
N1	C22	1.360(5)	C15	C21	1.396(7)
N2	C20	1.319(6)	C16	C17	1.338(7)
N2	C24	1.355(6)	C16	C21	1.440(6)
N3	C3	1.321(5)	C17	C23	1.458(7)
N4	C4	1.324(5)	C18	C19	1.339(8)
N5	C2	1.333(5)	C18	C23	1.402(7)
N5	C9	1.394(5)	C19	C20	1.409(7)
N5	C11	1.491(5)	C21	C22	1.402(6)
C1	C8	1.503(5)	C22	C24	1.434(6)
C2	C8	1.373(5)	C23	C24	1.409(6)

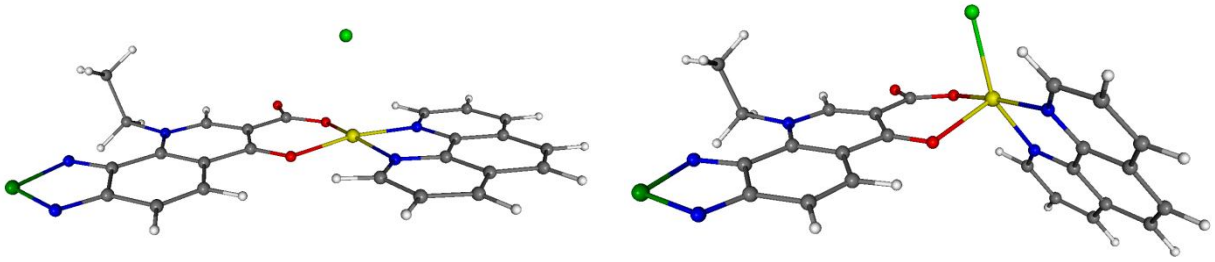
Table S6 Experimental (X-ray) bond angles of complex **3**

Atoms			Angle/°	Atoms			Angle/°
N3	Se1	N4	93.0(2)	C5	C6	C10	122.6(4)
O1	Cu1	Cl1	91.2(1)	O3	C7	C8	125.0(3)
O1	Cu1	O3	93.2(2)	O3	C7	C10	118.1(3)
O1	Cu1	N1	164.5(2)	C8	C7	C10	116.9(3)
O1	Cu1	N2	91.6(2)	C2	C8	C1	116.8(4)
O3	Cu1	Cl1	99.0(1)	C2	C8	C7	118.0(3)
O3	Cu1	N1	90.7(2)	C7	C8	C1	125.1(3)
O3	Cu1	N2	167.8(2)	N5	C9	C3	122.7(3)
N1	Cu1	Cl1	103.1(1)	C10	C9	N5	119.2(3)
N2	Cu1	Cl1	92.1(1)	C10	C9	C3	118.1(3)
N2	Cu1	N1	81.8(2)	C6	C10	C7	118.0(3)
C1	O1	Cu1	125.6(3)	C9	C10	C6	120.6(3)
C7	O3	Cu1	124.3(3)	C9	C10	C7	121.4(3)
C13	N1	Cu1	129.2(3)	N5	C11	C12	110.3(3)
C13	N1	C22	118.0(4)	N1	C13	C14	122.5(4)
C22	N1	Cu1	112.8(3)	C15	C14	C13	119.4(4)
C20	N2	Cu1	128.9(3)	C14	C15	C21	119.3(4)
C20	N2	C24	118.2(4)	C17	C16	C21	120.7(5)
C24	N2	Cu1	112.8(3)	C16	C17	C23	122.4(4)
C3	N3	Se1	107.9(3)	C19	C18	C23	120.5(4)
C4	N4	Se1	107.6(3)	C18	C19	C20	119.8(5)
C2	N5	C9	118.6(3)	N2	C20	C19	122.0(5)
C2	N5	C11	117.0(3)	C15	C21	C16	124.0(4)
C9	N5	C11	124.5(3)	C15	C21	C22	117.2(4)
O1	C1	C8	119.3(4)	C22	C21	C16	118.8(4)
O2	C1	O1	122.4(4)	N1	C22	C21	123.6(4)
O2	C1	C8	118.3(4)	N1	C22	C24	115.8(4)
N5	C2	C8	125.9(4)	C21	C22	C24	120.6(4)
N3	C3	C4	115.6(3)	C18	C23	C17	126.4(4)
N3	C3	C9	125.5(3)	C18	C23	C24	116.2(5)
C4	C3	C9	118.9(3)	C24	C23	C17	117.4(4)
N4	C4	C3	115.9(3)	N2	C24	C22	116.6(3)
N4	C4	C5	123.4(4)	N2	C24	C23	123.3(4)
C5	C4	C3	120.7(3)	C23	C24	C22	120.1(4)
C6	C5	C4	119.1(4)				



(A^{II}) (A^{OO}) (A^{OI})

Figure S1 Scheme of possible conformations of **A** with respect to the orientation of ethyl groups



(a) (b)

Figure S2: Optimized structure of complex **3**:(a) "planar" and (b) "non-planar" conformation

Table S7 Experimentally obtained (X-ray diffraction data) and calculated B3LYP/6-311G** (Calc.) bond distances in Å, and QTAIM BCP characteristics, *i.e.*, charge density ρ_{BCP}, Laplacian $\Delta\rho_{BCP}$ and delocalization indexes (DI) of Se-N bonds in studied complexes. A comparison to the selenadiazaquinolone-carboxylic acid (HE4*h*) is also given.

Distances /Å			**QTAIM analysis**		
1	X-ray	Calc. A^{OO} (B^{OO})	ρ_{BCP}/ bohr^{-3}	$\Delta\rho_{BCP}$/ bohr^{-5}	DI/ -
Se1-N3	1.807(4)	1.851 (1.803)	0.161 (0.177)	0.018 (0.025)	1.210 (1.274)
Se1-N4	1.796(5)	1.844 (1.801)	0.163 (0.177)	0.022 (0.038)	1.222 (1.268)
Se2-N6	1.793(4)	1.802 (1.803)	0.178 (0.177)	0.026 (0.025)	1.278 (1.274)
Se2-N7	1.781(5)	1.798 (1.801)	0.178 (0.177)	0.040 (0.038)	1.273 (1.268)
2		Calc. A^{OO} (B^{OO})			
Se1-N3	1.795(3)	1.804 (1.803)	0.177 (0.177)	0.025 (0.025)	1.274 (1.274)
Se1-N4	1.782(4)	1.801 (1.801)	0.177 (0.177)	0.038 (0.038)	1.268 (1.268)
Se2-N6	1.778(3)	1.802 (1.802)	0.177 (0.177)	0.025 (0.025)	1.274 (1.274)
Se2-N7	1.782(4)	1.799 (1.799)	0.177 (0.177)	0.038 (0.038)	1.268 (1.268)
3		Calc.			
Se-N3	1.784(3)	1.799	0.177	0.039	1.272
Se-N4	1.787(3)	1.802	0.178	0.026	1.277
HE4*h*					
Se-N3		1.799	0.177	0.038	1.271
Se-N4		1.802	0.178	0.025	1.278

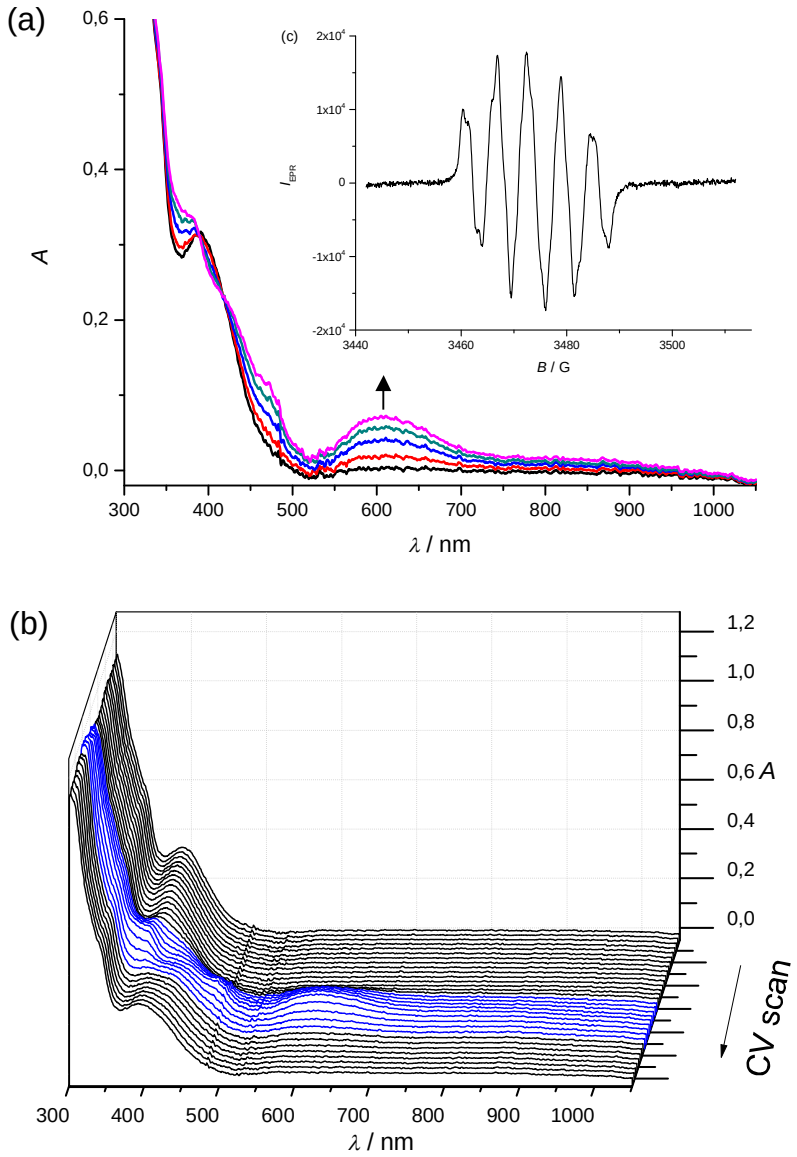


Figure S3. In situ EPR/UV-vis-NIR spectroelectrochemistry for **1** in DMSO/nBu_4NPF_6 (scan rate 10 mV s^{-1}): (a) UV-vis-NIR spectra detected simultaneously during the in situ reduction in the region of the first reduction double-peak (Inset: representative EPR spectrum of the ligand-centered radical measured upon cathodic reduction; (b) 3D presentation of the changes of optical bands measured in situ during cyclic voltammetry in the cathodic part.

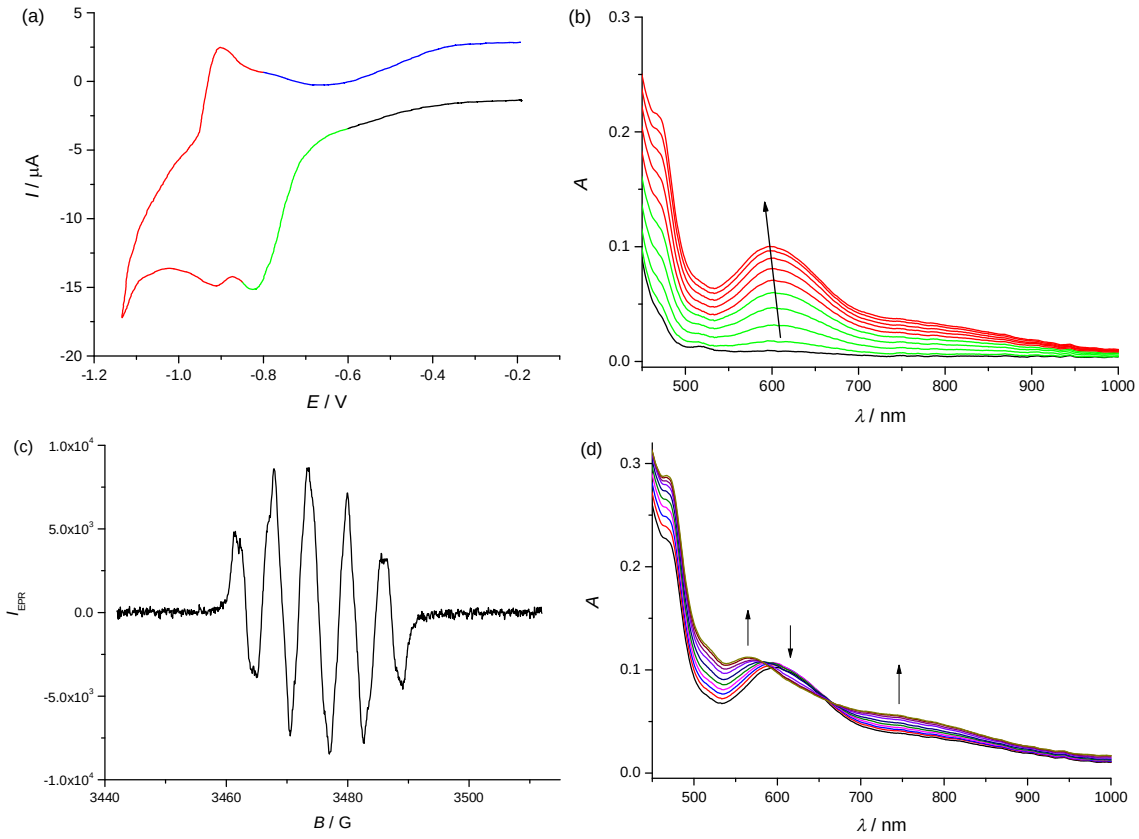


Figure S4 In situ EPR/UV-vis-NIR spectroelectrochemistry for **2** in DMSO/nBu_4NPF_6 (scan rate 10 mV s^{-1}): (a) the corresponding voltammogram with potential regions of the first and second peaks color highlighted; (b) UV-vis-NIR spectra detected simultaneously during the in situ reduction in the region of the first (green lines) and of the second peak (red lines). (c) representative EPR spectrum of the ligand-centered radical measured upon cathodic reduction of **2**; (d) UV–vis-NIR spectra detected during back scan at the second peak.

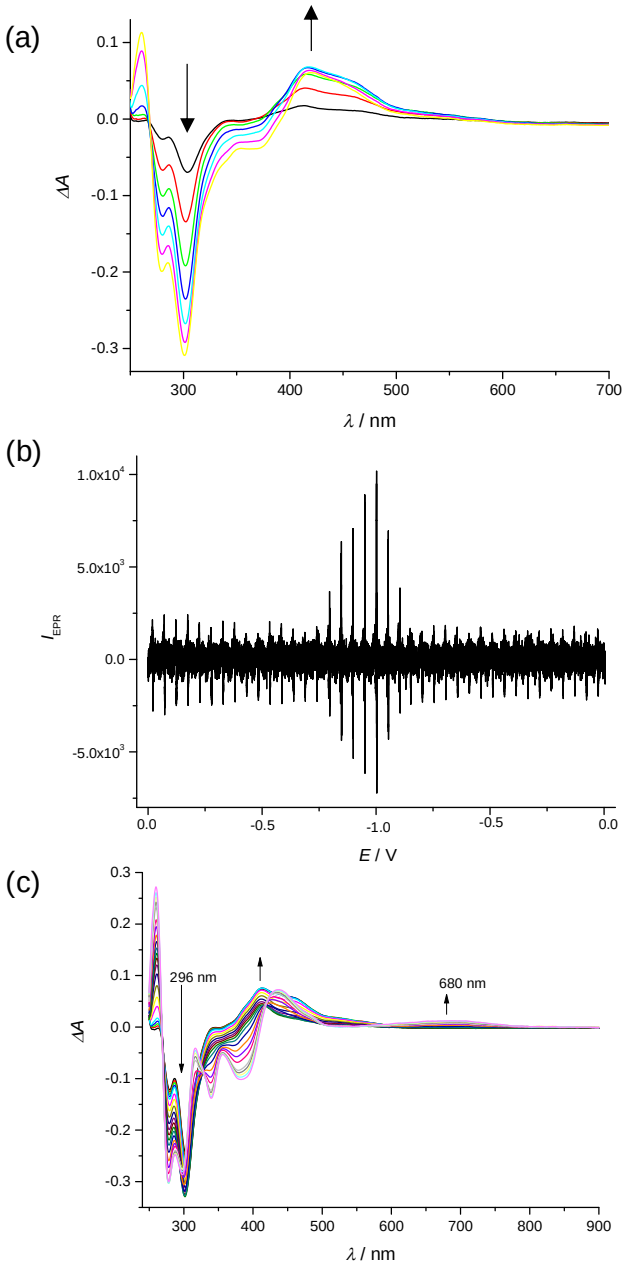


Figure S5 EPR and UV-Vis-NIR spectroelectrochemistry of complex **3** (a): Difference UV-vis-NIR spectra (initial sample solution was taken as reference) measured upon cathodic reduction of **3** in the region of the first reduction peak. (b): Potential dependence of EPR spectra measured in situ during cyclic voltammetry in the cathodic part. (c): Difference UV-vis-NIR spectra measured upon cathodic reduction of **3** in the region of the second reduction peak (in DMSO/nBu_4NPF_6).

Table S8 Contacts shorter than sum of van der Waals radii for complex **1**

Atom1	Atom2	Length	Length-VdW	Symm. op. 1	Symm. op. 2
H24A	H26	2.366	-0.034	x,y,z	1-x,-1/2+y,1/2-z
O1	H30	2.441	-0.279	x,y,z	-x,1-y,1-z
H29	O2A	2.692	-0.028	x,y,z	-x,1-y,1-z
H23B	N4	2.72	-0.030	x,y,z	-1+x,y,z
C17	H11A	2.788	-0.112	x,y,z	-1+x,y,z
C24	H26	2.87	-0.030	x,y,z	1-x,-1/2+y,1/2-z
Se2	H12A	2.996	-0.104	x,y,z	1-x,-y,1-z
Se1	N7	3.012	-0.438	x,y,z	1-x,-y,1-z
C31	C25	3.333	-0.067	x,y,z	-1+x,y,z
C21	C4	3.362	-0.038	x,y,z	-1+x,y,z
C29	C32	3.379	-0.021	x,y,z	-x,1-y,1-z
C30	C36	3.386	-0.014	x,y,z	-x,1-y,1-z
C15	Se1	3.488	-0.112	x,y,z	-1+x,y,z
Se2	C12	3.571	-0.029	x,y,z	1-x,-y,1-z
Se2	Se1	3.635	-0.165	x,y,z	-1+x,y,z

Table S9 Contacts shorter than sum of van der Waals radii for complex **2**

Atom1	Atom2	Length	Length-VdW	Symm. op. 1	Symm. op. 2
O1	H30	2.539	-0.181	x,y,z	-x,1-y,1-z
H29	O2A	2.647	-0.073	x,y,z	-x,1-y,1-z
C17	H11A	2.843	-0.057	x,y,z	-1+x,y,z
H31	C1A	2.872	-0.028	x,y,z	-1+x,y,z
Se1	N7	3.081	-0.369	x,y,z	1-x,-y,1-z
C31	C25	3.372	-0.028	x,y,z	-1+x,y,z
C15	Se1	3.527	-0.073	x,y,z	-1+x,y,z
Se2	Se1	3.738	-0.062	x,y,z	-1+x,y,z

Table S10 Contacts shorter than sum of van der Waals radii for complex **3**

Atom1	Atom2	Length	Length-VdW	Symm. op. 1	Symm. op. 2
Cl1	H13	2.865	-0.085	x,y,z	-x,1-y,1-z
Cl1	H6	2.906	-0.044	x,y,z	-x,1-y,1-z
N4	N4	2.928	-0.172	x,y,z	-x,-y,1-z
Cl1	H14	2.936	-0.014	x,y,z	-x,1-y,1-z
Se1	N4	2.986	-0.464	x,y,z	-x,-y,1-z
C10	C24	3.389	-0.011	x,y,z	1-x,1-y,1-z
C4	C18	3.397	-0.003	x,y,z	1-x,1-y,1-z
C5	C19	3.398	-0.002	x,y,z	1-x,1-y,1-z