Electronic Supplementary Material (ESI) for New Journal of Chemistry.

New cobalt(II) coordination designs and influence of varying chelate characters, ligand charges and incorporated group I metal ion on enzyme-like oxidative coupling activity

Supporting Information

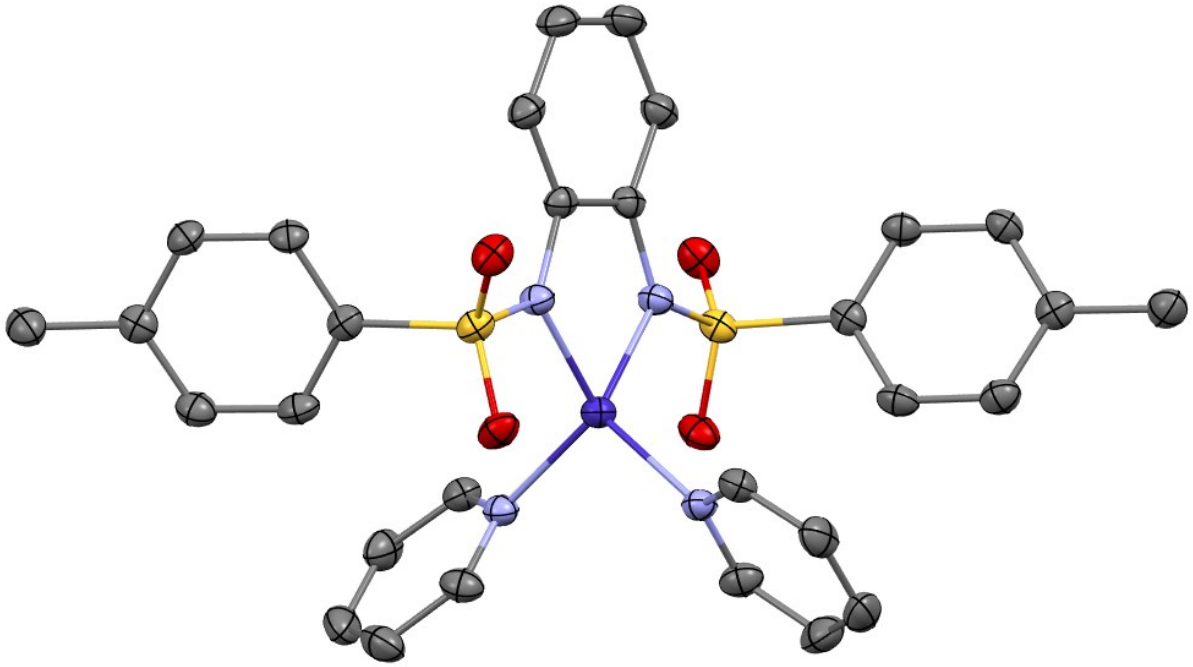


Fig. S1: Molecular structure of the mixed ligand complex **Co2** bearing the dianionic ligand **2** and two pyridine co-ligands. Some atomic labels and protons are omitted for clarity.

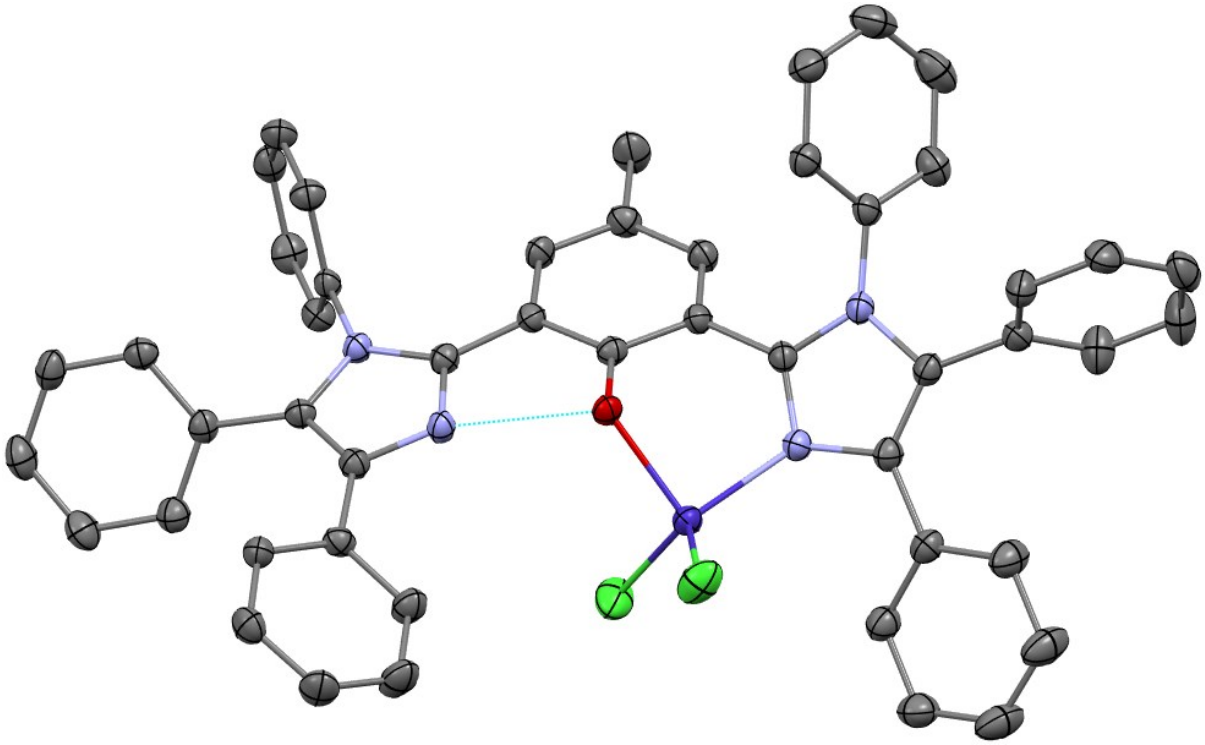


Fig. S2: Molecular structure of **Co3** with thermal ellipsoids drawn at the 50% probability level. Some atomic labels and protons have been omitted for clarity.

Table S1: Structural refinement data for the studied complexes

Compound	(Na-**CoL**-*i*)$_2$	(Na-**CoL**-e)$_2$	(K-**CoL**-e)$_2$	(Cs-**CoL**-e)$_2$
formula	$C_{94}H_{130}Co_2N_8$ $Na_2O_{14}S_4$	$C_{92}H_{124}Co_2N_8Na_2O_{14}S_4$ [*]	$C_{92}H_{130}Co_2K_2N_8O_{16}S_4$ [*]	$C_{98}H_{150}Co_2Cs_2N_8O_{20}S_4$
fw (g·mol^{-1})	1888.13	1858.06 [*]	1928.33 [*]	2272.17
T/°*C*	-140(2)	-140(2)	-140(2)	-140(2)
crystal system	monoclinic	Triclinic	Triclinic	triclinic
space group	'P 21/n'	'P -1'	'P -1'	'P -1'
a/ Å	11.2513(3)	14.6152(4)	14.0537(3)	14.3365(3)
b/ Å	15.5659(4)	14.7527(4)	14.4047(2)	14.3483(4)
c/ Å	29.1361(8)	15.6217(5)	15.4849(3)	15.5549(4)
α/°	90	71.507(1)	83.385(1)	83.193(1)
β/°	100.708(1)	82.660(2)	70.121(1)	70.741(1)
γ/°	90	64.815(1)	68.089(1)	68.091(1)
V/Å^3	5013.9(2)	2890.57(15)	2734.77(9)	2802.45(12)
Z	2	1	1	1
ρ (g·cm^{-3})	1.251	1.067 [*]	1.171 [*]	1.346
μ (cm^{-1})	4.85	4.20 [*]	5.14 [*]	10.75
measured data	24143	35063	27162	25640
data with I > 2σ(I)	9650	9545	10809	10092
unique data (R_{int})	10918/0.0537	13062/0.0422	12421/0.0254	12709/0.0382
wR_2 (all data, on F^2)[a)]	0.1273	0.2397	0.1560	0.1464
R_1 ($I > 2\sigma(I)$) [a)]	0.0536	0.0901	0.0592	0.0673
S [b)]	1.147	1.039	1.107	1.041
Res. dens./e·Å^{-3}	0.517/-0.689	2.058/-1.033	1.644/-2.381	1.341/-1.162
absorpt method	multi-scan	multi-scan	multi-scan	multi-scan
absorpt corr $T_{min/max}$	0.5783/0.7456	0.6623/0.7456	0.6985/0.7456	0.6792/0.7456
CCDC No.	1986221	1986222	1986223	1986224

[*] derived parameters do not contain the contribution of the disordered solvent.

[a)] Definition of the *R* indices: $R_1 = (\Sigma \,||F_o| - |F_c||)/\Sigma |F_o|$;

$wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ with $w^{-1} = \sigma^2(F_o^2) + (aP)^2+bP$; $P = [2F_c^2 + \mathrm{Max}(F_O^2)]/3$;

[b)] $s = \{\Sigma[w(F_o^2-F_c^2)^2]/(N_o-N_p)\}^{1/2}$.

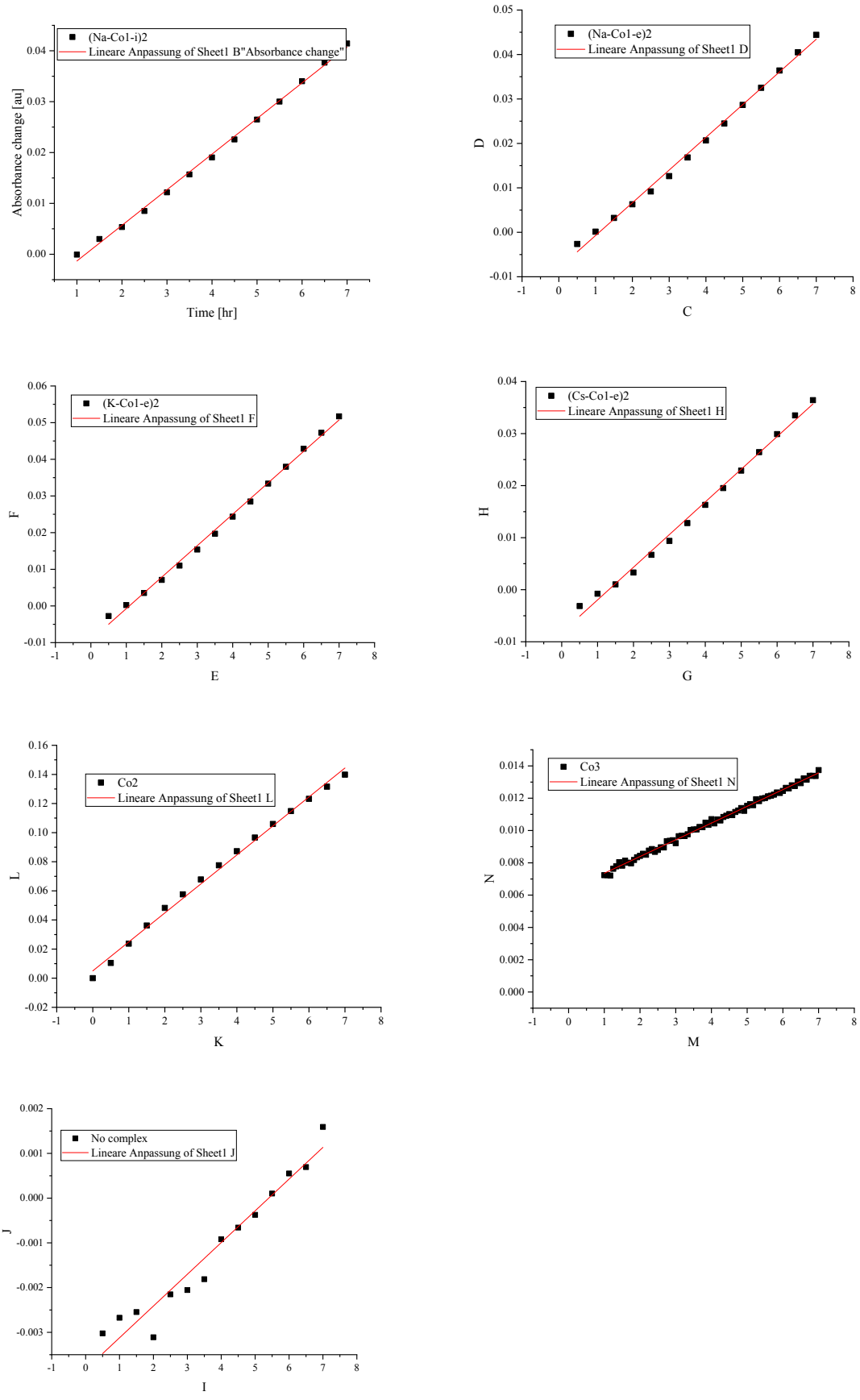
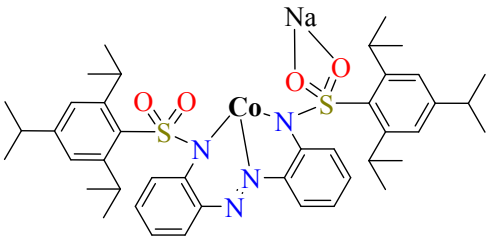
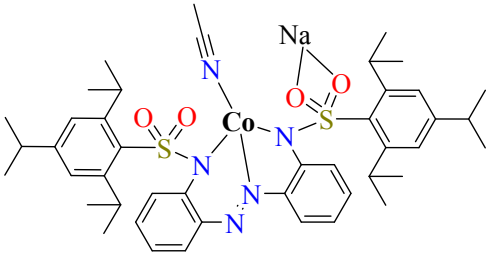


Fig. S3: Linear fitting of absorbance change with time

ESI-MS +ve Mode



Molecular Weight: 824,96



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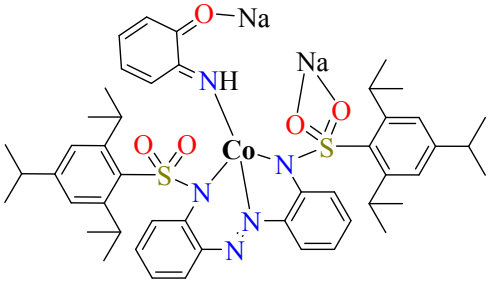

Molecular Weight: 955,06

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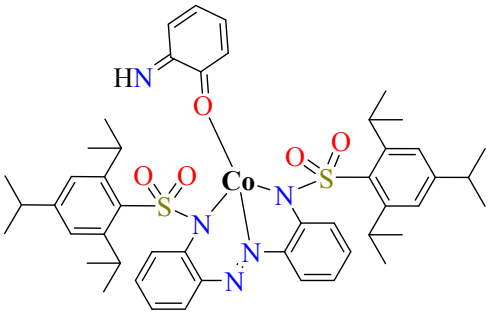

Molecular Weight: 909,08

Fig. S4: UV-Vis. Data of the studied complexes