Electronic Supplementary Information for the *New Journal of Chemistry* article:

Necessity of free and uncrowded coordination environments in biomimetic complex models: oxidative coupling by mixed-ligand cobalt(II) complexes of diazene-disulfonamide

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Table S1: Crystal data and refinement details for the X-ray structure determinations of the compounds **Co1(*im*)$_2$**, **Co1(*py*)$_2$**, **Co2(*im*)$_2$** and **Co2(*py*)$_2$**.

Compound	**Co1(*im*)$_2$**	**Co1(*py*)$_2$**	**Co2(*im*)$_2$**	**Co2(*py*)$_2$**
formula	$C_{22}H_{26}CoN_8O_4S_2$	$C_{24}H_{24}CoN_6O_4S_2$	$C_{34}H_{34}CoN_8O_4S_2$	$C_{37}H_{36}CoN_6O_5S_2$
fw (g·mol^{-1})	589.56	583.54	741.74	767.77
°C	-140(2)	-140(2)	-140(2)	-140(2)
crystal system	monoclinic	monoclinic	triclinic	orthorhombic
space group	P 2_1/n	P 2_1/n	P $\bar{1}$	P n a 2_1
a/ Å	9.2768(2)	16.8164(4)	9.2159(2)	25.0084(5)
b/ Å	14.5362(4)	9.0073(2)	12.0557(4)	9.5461(2)
c/ Å	56.2278(11)	18.1311(4)	16.1593(5)	14.8410(3)
α/°	90	90	90.159(3)	90
β/°	94.518(3)	113.839(1)	105.367(3)	90
γ/°	90	90	105.575(1)	90
V/Å^3	7558.7(3)	2512.02(10)	1662.32(8)	3543.03(13)
Z	12	4	2	4
ρ (g·cm^{-3})	1.554	1.543	1.482	1.439
μ (cm^{-1})	8.94	8.94	6.95	6.55
measured data	48191	16961	20848	41560
data with I > 2σ(I)	14996	4813	5203	6855
unique data (R_{int})	17083/0.0282	5710/0.0458	7540/0.0626	8081/0.0538
wR_2 (all data, on F^2)[a]	0.0773	0.0982	0.1424	0.1071

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R_1 ($I > 2\sigma(I)$) [a]	0.0320	0.0450	0.0692	0.0486
S [b]	1.041	1.025	1.076	1.060
Res. dens./e·Å^{-3}	0.412/-0.421	1.115/-0.830	0.709/-0.479	1.126/-0.387
Flack-parameter	-	-	-	0.124(16)
absorpt method	multi-scan	multi-scan	multi-scan	multi-scan
absorpt corr $T_{min}/_{max}$	0.6748/0.7456	0.6813/0.7456	0.6545/0.7456	0.7001/0.7456
CCDC No.	1894914	1894915	1894916	1894917

[a] Definition of the R indices: $R_1 = (\Sigma \mid\mid F_o \mid - \mid F_c \mid\mid)/\Sigma \mid F_o \mid$; $wR_2 = \{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$ with $w^{-1} = \sigma^2(F_o^2) + (aP)^2+bP$; $P = [2F_c^2 + Max(F_O^2]/3$;
[b] $S = \{\Sigma[w(F_o^2-F_c^2)^2]/(N_o-N_p)\}^{1/2}$.

Table S2: Minimal distortion path analysis from vOC-5 (0 %) to TBPY-5 (100 %) for **Co1(*py*)$_2$** and **Co2(*py*)$_2$**

	Co1(*py*)$_2$	**Co2(*py*)$_2$**
$S(C_{4v})$	1.574	2.079
$S(D_{3h})$	3.598	2.752
DevPath	15.4	13.5
Gencoord	-	-

vOC-5 (C_{4v}) Vacant octahedron, TBPY-5 (D_{3h}) Trigonal bipyramid, DevPath (Path Deviation), Gencoord (Generalized coordinate), Deviation threshold to calculate Generalized Coordinate: 10.000%

Table S3: Bond angles in the square plane of the coordination compsounds:

Bond angles (Å)				
	Co1(*im*)$_2$	**Co1(*py*)$_2$**	**Co2(*im*)$_2$**	**Co2(*py*)$_2$**
N1−Co1–N4	169.70 (6)	170.02 (9)	169.41 (13)	168.60 (14)
N6/N7−Co1–N5	164.66 (6)	160.37 (10)	166.80 (13)	156.19 (11)

Table S4: Temperature effect on the phenoxazinone mimicking activity of **Co1(*dpy*)$_2$**

Temp. (°C)	**Initial rate (× 10^{-3} h^{-1})**
25	58.22
35	84.61
45	130.29
55	159.86

65	189.58

Reaction conditions: Solvent (acetonitrile), catalyst (5×10^{-5} M), OAPH (5×10^{-3} M), temperature (25 – 65 ^{o}C).