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ELECTRONIC SUPPORTING INFORMATION

New Heteroleptic bis-(diphenylphosphino)ethane appended dialkyldithiophosphatecobalt(III) cations: Apt electrocatalysts for heterogeneous OER and homogeneous HER

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Fig. S1 Electronic absorption spectrum of Co-Et and Co-Pr in 1×10^{-4} M dichloromethane solution.



Fig. S2 FESEM images for (a) and (c) Pristine **Co-Et** and **Co-Pr**, respectively; (b) and (d) **Co-Et** and **Co-Pr** after OER electrocatalysis in 0.1 M KOH.



Fig. S3 XPS spectra for (a) Co-Et and (b) Co-Pr before and after OER electrocatalysis.



Fig. S4 Linear sweep votammograms for Co-Et and Co-Pr in 0.5 M H₂SO₄.



Fig. S5 The UV-Vis spectra for Co-Et+TFA recorded in acetonitrile at zero time and after 3 h.



Fig. S6 The UV-Vis spectra for Co-Pr+TFA recorded in acetonitrile at zero time and after 3 h.



Fig. S7 Linear sweep voltammograms for **Co-Et** recorded at different scan rates in 0.1 M KOH solution.



Fig. S8 Linear sweep voltammograms for **Co-Pr** recorded at different scan rates in 0.1 M KOH solution.

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Table	S1.	Comparison	of	electrocatalytic	behavior	of	different	Cobalt	based	coordination
compl	exes	towards OER	•							

	Current	Overpotential	Tafel Slope	Ref
	density	(in V)	(mV/dec)	
	(mA/cm^2)			
$[Co(OH_2)_2(PMBP)_2](1)$	10	0.140	50	1
$[Co(OH_2)_2(PMTP)_2]$ (2)	10	0.320	90	1
$([Co1.5(tib)(dcpna)] \cdot 6H_2O)$	10	0.360	89	2
$[CoL_2)$ (H ₂ L = 4-chloro-1,2-bis [2-hydroxy-5-	10	0.360	-	3
(phenylazo)benzylideneamino]benzene				
[CoL ₂] L ₂ :Bis[Salicylydene]-1,2-	2	0.140	84	3
Iminophenylenediamine				
[Co(L)(CHOH)]	0.5	0.520	-	3
L: Soduim (E)-4-(2-				
hydroxylnaphtalene-1-yl)diazinyl	5	0.720	-	3
benzenesulfonate				
$[\mathrm{Co}^{\mathrm{III}}(\mathrm{LN}_{2}\mathrm{O}_{3})\mathrm{H}_{2}\mathrm{O}]$	10	0.500	-	4
Co-Et	10	0.672	114	This
				work
Co-Pr	10	0.724	151	This
				work

References

- 1. C. S. A. Djadock, S. Vengatesan, A. C. T. Kuate, J. Ngoune, S. Ravichandrana and S. Vasudevan, *Catal. Sci. Technol.*, 2023, 13, 2184-2200.
- 2. M. Qingguo, Y. Jianjian, M. Shixuan, Z. Mujun and L. Jitao, Polymers, 2017, 9, 676.
- 3. Z. Xiaoxin, H.Xiaoxi, G. Anandarup, S. Rafael, R. S. Bhaskar, M. Eliska, and A. Tewodros, *Angew. Chem. Int. Ed.*, 2014, 126, 4461–4465.
- X. Zhicai, L. Qian, X. Wei, M. A. Abdullah, S. Xuping, Chem. Sus. Chem., 2015, 8(11), 1850– 1855.