

ESI to accompany

Influence of a co-adsorbant on the performance of bis(diimine) copper(I)-based dye-sensitized solar cells

Sven Y. Brauchli,^a Frederik J. Malzer,^a Edwin C. Constable^{*a} and Catherine E. Housecroft^{*a}

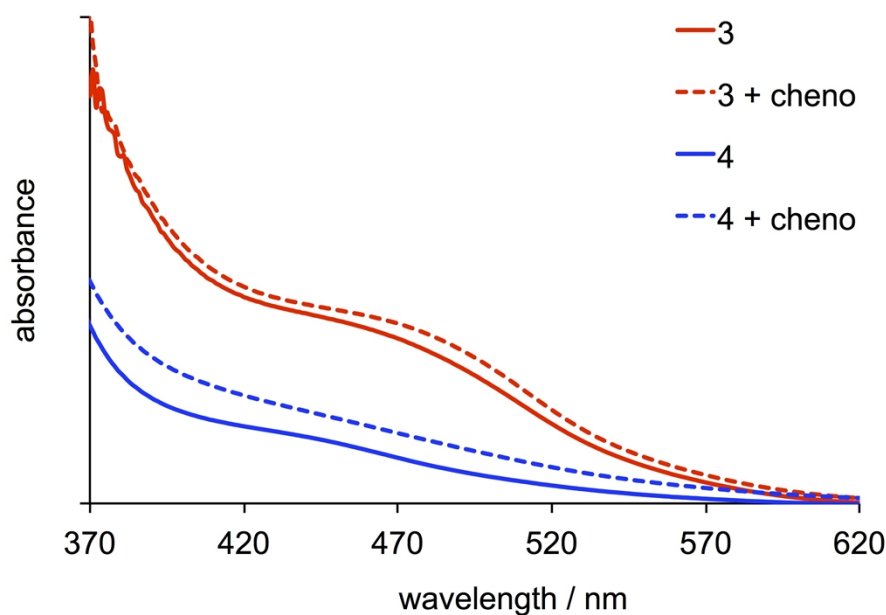


Fig. S1. Solid-state absorption spectra of electrodes (without scattering layer) with the anchored second-generation dyes $[\text{Cu}(\mathbf{1})(\mathbf{3})]^+$ (methyl substituents in **3**) and $[\text{Cu}(\mathbf{1})(\mathbf{4})]^+$ (phenyl substituents in **4**) with and without cheno. CH_2Cl_2 was the solvent used in the dye-bath.

Table S1. DSC performance data for masked cells using the dyes [Cu(1)(3)]⁺ and [Cu(1)(4)]⁺ with cheno as co-adsorbant. Relative efficiencies (last column) are with respect to 100% for dye N719 measured under the same conditions. V_{oc} = open circuit voltage, J_{sc} = short circuit current density, ff = fill factor.

Anchored dye	Additive	Solvent	J_{sc} / mA cm ⁻²	V_{oc} / mV	ff / %	η / %	Rel. η / %
On the day of sealing the cells							
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	6.07	530	70.8	2.28	28.6
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	6.02	531	69.6	2.23	28.0
[Cu(1)(3)] ⁺	cheno	acetone	5.55	485	41.8	1.12	14.1
[Cu(1)(3)] ⁺	cheno	acetone	6.72	520	60.9	2.13	26.8
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	4.19	511	67.8	1.45	18.2
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	3.74	493	67.1	1.24	15.6
[Cu(1)(4)] ⁺	cheno	acetone	6.27	536	69.6	2.34	29.4
[Cu(1)(4)] ⁺	cheno	acetone	6.34	546	70.8	2.45	30.8
N719		ethanol	16.73	669	71.2	7.96	100
1 day after sealing the cells							
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	5.56	530	72.2	2.12	25.8
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	5.70	551	71.3	2.24	27.3
[Cu(1)(3)] ⁺	cheno	acetone	5.71	493	44.4	1.25	15.2
[Cu(1)(3)] ⁺	cheno	acetone	6.26	532	62.6	2.09	25.4
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	4.18	525	69.3	1.52	18.5
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	3.91	522	69.2	1.41	17.2
[Cu(1)(4)] ⁺	cheno	acetone	6.13	542	69.9	2.32	28.2
[Cu(1)(4)] ⁺	cheno	acetone	6.16	551	71.0	2.41	29.3
N719		ethanol	16.72	685	71.7	8.22	100
2 days after sealing the cells							
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	5.76	550	72.0	2.28	27.0
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	5.88	562	71.7	2.37	28.0
[Cu(1)(3)] ⁺	cheno	acetone	5.67	507	43.4	1.25	14.8
[Cu(1)(3)] ⁺	cheno	acetone	6.14	528	64.0	2.08	24.6
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	4.40	532	69.1	1.62	19.2
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	4.28	522	69.7	1.55	18.3
[Cu(1)(4)] ⁺	cheno	acetone	5.96	549	70.1	2.30	27.2
[Cu(1)(4)] ⁺	cheno	acetone	6.25	554	71.0	2.45	29.0
N719		ethanol	16.87	698	71.7	8.45	100
15 days after sealing the cells							
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	5.64	576	72.5	2.36	28.1
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	5.96	575	71.1	2.43	28.9
[Cu(1)(3)] ⁺	cheno	acetone	5.32	511	49.3	1.34	15.9
[Cu(1)(3)] ⁺	cheno	acetone	5.94	540	64.7	2.07	24.6
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	4.74	554	69.2	1.82	21.6
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	4.53	549	69.8	1.74	20.7
[Cu(1)(4)] ⁺	cheno	acetone	6.10	564	64.7	2.23	26.5
[Cu(1)(4)] ⁺	cheno	acetone	6.34	551	70.9	2.48	29.5
N719		ethanol	16.52	704	72.3	8.41	100
22 days after sealing the cells							
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	5.86	566	71.4	2.36	28.7
[Cu(1)(3)] ⁺	cheno	CH ₂ Cl ₂	6.18	572	70.0	2.47	30.0
[Cu(1)(3)] ⁺	cheno	acetone	4.76	522	42.6	1.06	12.9
[Cu(1)(3)] ⁺	cheno	acetone	6.27	553	60.1	2.08	25.3
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	5.02	553	67.9	1.89	23.0
[Cu(1)(4)] ⁺	cheno	CH ₂ Cl ₂	4.95	555	68.3	1.87	22.7
[Cu(1)(4)] ⁺	cheno	acetone	6.36	569	63.4	2.30	28.0
[Cu(1)(4)] ⁺	cheno	acetone	6.33	552	70.9	2.48	30.2

N719		ethanol	16.34	704	71.4	8.22	100
------	--	---------	-------	-----	------	------	-----

Table S2. Performance data of duplicate DSCs (cells 1 and 2) with [Cu(1)(5)]⁺, cheno being introduced with ancillary ligand 5 and [Cu(MeCN)₄]⁺; data are compared to a DSC containing N719 measured under the same conditions. The parameters for cell 1 are given in Table 3 of the main paper.

Dye	Cell number	Ratio of [Cu(MeCN) ₄] ⁺ : 5 : cheno in dye bath	On the day of sealing the cell				
			$J_{sc} /$ mA cm ⁻²	$V_{oc} /$ mV	$ff /$ %	$\eta /$ %	Relative $\eta /$ %
[Cu(1)(5)] ⁺	1	1 : 1 : 1	6.74	573	69.7	2.69	41.5
	2	1 : 1 : 1	6.41	569	71.3	2.60	40.1
[Cu(1)(5)] ⁺	1	1 : 1 : 3	5.66	563	73.0	2.33	36.0
	2	1 : 1 : 3	4.57	580	71.7	1.90	29.3
[Cu(1)(5)] ⁺	1	1 : 1 : 6	6.27	568	72.1	2.57	39.7
	2	1 : 1 : 6	6.29	575	71.6	2.59	40.0
[Cu(1)(5)] ⁺	1	1 : 1 : 10	6.48	564	70.6	2.58	39.8
	2	1 : 1 : 10	6.15	576	71.6	2.54	39.2
N719			16.55	636	61.6	6.48	100
3 days after sealing the cell							
			$J_{sc} /$ mA cm ⁻²	$V_{oc} /$ mV	$ff /$ %	$\eta /$ %	Relative $\eta /$ %
[Cu(1)(5)] ⁺	1	1 : 1 : 1	6.78	574	69.8	2.71	37.7
	2	1 : 1 : 1	6.47	583	71.1	2.68	37.3
[Cu(1)(5)] ⁺	1	1 : 1 : 3	6.36	593	70.1	2.64	36.7
	2	1 : 1 : 3	5.33	611	69.6	2.26	31.4
[Cu(1)(5)] ⁺	1	1 : 1 : 6	6.56	584	72.0	2.76	38.4
	2	1 : 1 : 6	6.22	583	71.0	2.57	35.7
[Cu(1)(5)] ⁺	1	1 : 1 : 10	6.82	586	71.0	2.83	39.4
	2	1 : 1 : 10	6.65	602	70.7	2.83	39.4
N719			16.35	675	65.1	7.19	100
7 days after sealing the cell							
			$J_{sc} /$ mA cm ⁻²	$V_{oc} /$ mV	$ff /$ %	$\eta /$ %	Relative $\eta /$ %
[Cu(1)(5)] ⁺	1	1 : 1 : 1	6.84	571	69.8	2.72	36.1
	2	1 : 1 : 1	6.59	581	71.3	2.73	36.3
[Cu(1)(5)] ⁺	1	1 : 1 : 3	6.33	590	69.2	2.59	34.4
	2	1 : 1 : 3	5.28	605	71.8	2.29	30.4
[Cu(1)(5)] ⁺	1	1 : 1 : 6	6.47	581	73.1	2.75	36.5
	2	1 : 1 : 6	6.21	579	71.5	2.57	34.1
[Cu(1)(5)] ⁺	1	1 : 1 : 10	6.82	584	71.2	2.84	37.7
	2	1 : 1 : 10	6.75	600	69.0	2.80	37.2
N719			16.16	677	68.8	7.53	100

Table S3. Performance data of duplicate DSCs (cells 1 and 2) with [Cu(1)(5)]⁺, cheno being introduced with anchoring ligand 1; data are compared to a DSC containing N719 and measured under the same conditions. The parameters for cell 1 are given in Table 4 of the main paper.

Dye	Cell number	Ratio of 1 : cheno	On the day of sealing the cell				
			$J_{SC} /$ mA cm^{-2}	V_{OC} / mV	$ff / \%$	$\eta / \%$	Relative $\eta / \%$
[Cu(1)(5)] ⁺	1	1 : 1	5.43	566	68.9	2.12	28.0
	2	1 : 1	5.20	561	67.6	1.97	26.0
[Cu(1)(5)] ⁺	1	1 : 3	5.92	558	67.7	2.23	29.4
	2	1 : 3	5.68	556	69.3	2.19	28.9
[Cu(1)(5)] ⁺	1	1 : 6	5.73	536	68.8	2.11	27.8
	2	1 : 6	5.43	526	68.0	1.94	25.6
N719			16.18	656	71.4	7.58	100
3 days after sealing the cell							
			$J_{SC} /$ mA cm^{-2}	V_{OC} / mV	$ff / \%$	$\eta / \%$	Relative $\eta / \%$
[Cu(1)(5)] ⁺	1	1 : 1	6.02	570	70.0	2.40	31.6
	2	1 : 1	5.87	552	69.1	2.24	29.5
[Cu(1)(5)] ⁺	1	1 : 3	6.45	538	69.1	2.39	31.4
	2	1 : 3	6.18	541	69.7	2.33	30.7
[Cu(1)(5)] ⁺	1	1 : 6	5.79	562	70.1	2.28	30.0
	2	1 : 6	5.63	561	68.9	2.17	28.6
N719			16.18	671	70.0	7.60	100
7 days after sealing the cell							
			$J_{SC} /$ mA cm^{-2}	V_{OC} / mV	$ff / \%$	$\eta / \%$	Relative $\eta / \%$
[Cu(1)(5)] ⁺	1	1 : 1	6.15	574	70.7	2.49	31.5
	2	1 : 1	6.03	570	70.2	2.42	30.6
[Cu(1)(5)] ⁺	1	1 : 3	6.59	547	70.0	2.52	31.9
	2	1 : 3	6.60	551	70.3	2.55	32.2
[Cu(1)(5)] ⁺	1	1 : 6	5.75	564	70.0	2.27	28.7
	2	1 : 6	5.64	563	68.4	2.17	27.4
N719			16.14	697	70.4	7.91	100