

Supplementary Material

1,2,5-Thiadiazolo[3,4-*b*]pyrazine-5,6-dicarbonitrile and porphyrazines on its basis: synthesis and electrochemical study

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IR spectrum of dinitrile **2**

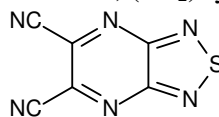
MALDI mass-spectra of porphyrazine **4**

Table 1S. Reduction potentials ($E_{1/2}$, eV) for pyrazine-2,3-dicarbonitriles and related π -acids containing 1,2,5-thiadiazole, pyrazine rings and/or cyano groups.

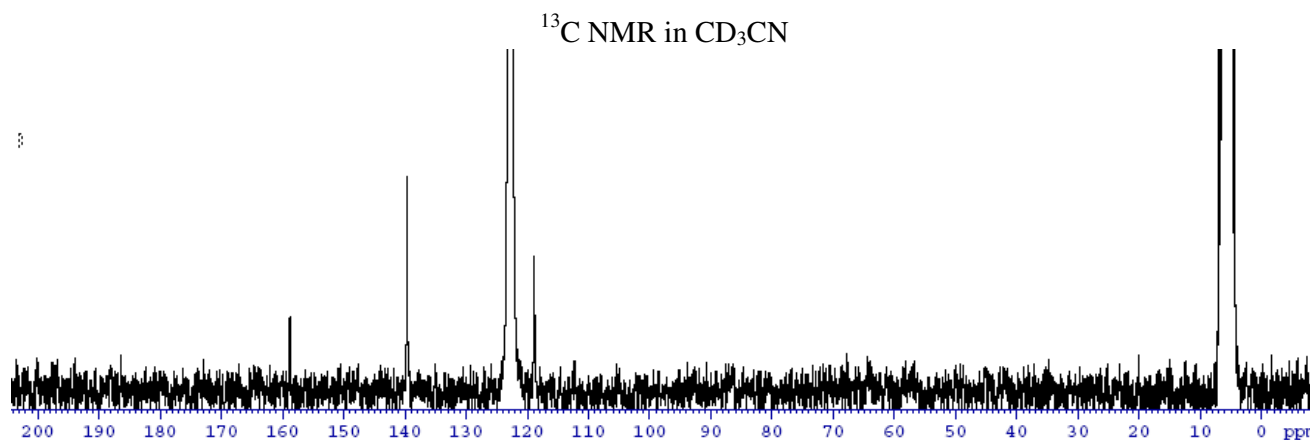
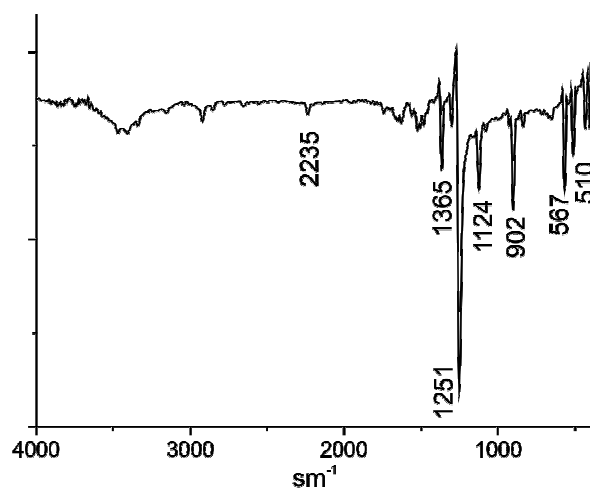
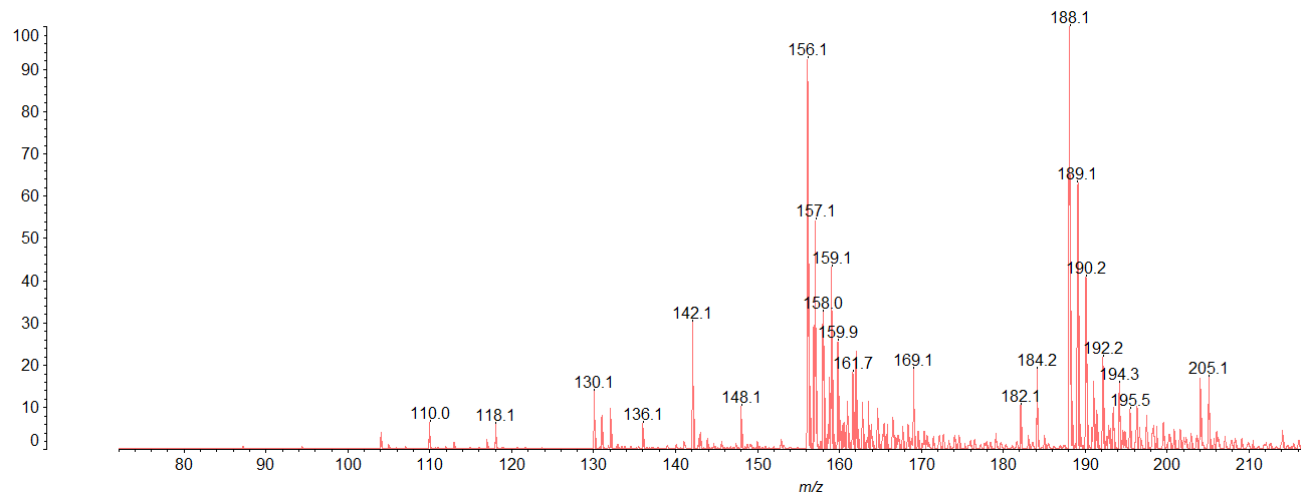
Dinitrile or π -acid	solvent	1 st reduction	2 nd reduction	Electrode	Ref. ^b
(SN ₂)(Pyz)(CN) ₂ (2)	MeCN	-0.01 / -0.05 ^a	-1.02	Ag/AgCl	this work
	DMSO	+0.08 / +0.03 ^a	-0.52, -0.72	Ag/AgCl	This work
(2-Fur) ₂ (Pyz)(Pyz)(CN) ₂	DMF	-0.25	-0.95	SCE	19
(2-Th) ₂ (Pyz)(Pyz)(CN) ₂	DMF	-0.25	-0.88	SCE	19
(2-Py) ₂ (Pyz)(Pyz)(CN) ₂	DMF	-0.25	-0.65	SCE	19
(^t BuPh) ₂ (Pyz)(Pyz)(CN) ₂	MeCN	-0.22 / +0.20 ^a		Fc/Fc+	17
(^t BuPh) ₂ (Bz)(Pyz)(CN) ₂	MeCN	-0.62 / -0.20 ^a		Fc/Fc+	17
(^t BuPh) ₂ (Pyz)(Bz)(CN) ₂	MeCN	-0.81 / -0.39 ^a		Fc/Fc+	17
(Py) ₂ (Pyz)(Bz)(CN) ₂	DMSO	-0.88	-1.66	SCE	23
(Cl ₂ Pt)(Py) ₂ (Pyz)(Bz)(CN) ₂	DMSO	-0.63	-1.37	SCE	23
(Me ⁺ Py) ₂ (Pyz)(CN) ₂		-0.36	-0.57	SCE	22
(Cl ₂ Pt)(Py) ₂ (Pyz)(CN) ₂	DMSO	-0.60	-1.25	SCE	22
Py ₂ (Pyz)(CN) ₂	Py	-0.93	-1.80	SCE	22
	DMSO	-0.87	-1.72	SCE	22
Ph ₂ (Pyz)(CN) ₂	Py	-1.05	-1.92	SCE	22
(Pyz)(CN) ₂	Py	-1.09	-1.54	SCE	22
(Pyz)(CN) ₄	CH ₂ Cl ₂	-0.23	-0.73	SCE	30
(SN ₂)(Pyz)	MeCN	-0.83	-1.82	SCE	27
(SN ₂)(Pyz)(SN ₂)	MeCN	+0.10	-0.82	SCE	28
(SN ₂)(Pyz)(Bz)	MeCN	-0.46		SCE	28
(SN ₂)(Pyz)(Cl) ₂	MeCN	-0.56		SCE	28
(SN ₂)C ₂ (CN) ₂	MeCN	-1.07		SCE	29
(SN ₂)TCNQ	MeCN	+0.12	-0.38	SCE	25
(SN ₂)TCNQ(SN ₂)	MeCN	-0.02	-0.49	SCE	25
TCNQ	MeCN	+0.08	-0.48	SCE	24
TCNE		+0.15			

^a Values corrected vs SCE using reference electrode corrections -0.045 v for Ag/AgCl, and +0.425 V for Fc+/Fc.³¹

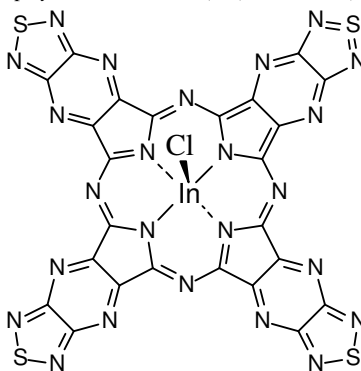
^b References are given in the main text

1,2,5-Thiadiazolo[3,4:5,6]pyrazine-2,3-dicarbonitrile, (SN₂)Pyz(CN)₂ (2)**2**

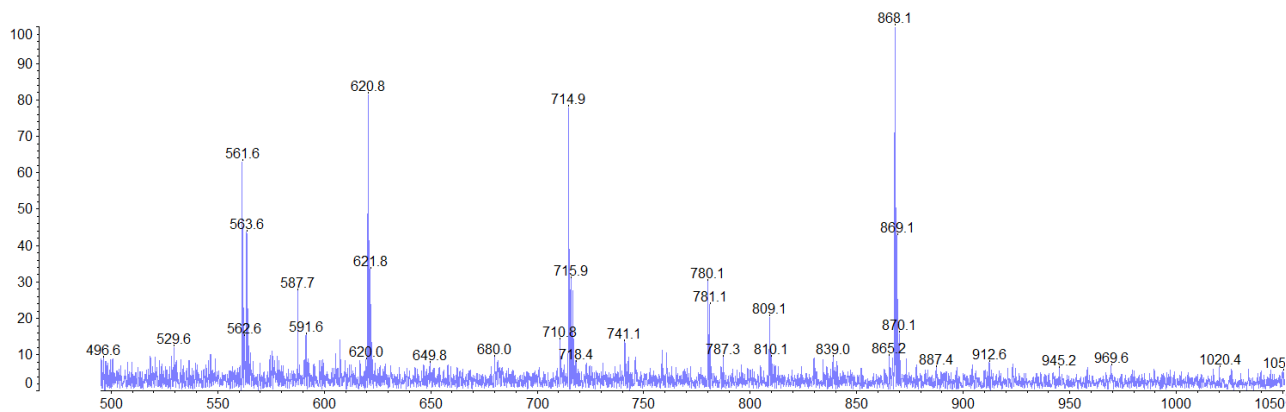
Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Reflectron_neg, Power: 50, Blanked, P.Ext. @ 700 (bin 58)
%Int. 809 mV[sum= 404466 mV] Profiles 1-500 Smooth Av 5 -Baseline 20



Tetrakis(1,2,5-thiadiazolo[3,4:5,6]pyrazino)porphyrzinatoindium(III) chloride (4), [T(SN₂Pyz)PAlnCl].



Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Reflectron_neg, Power: 85, Blanked, P.Ext. @ 400 (bin 58)
%Int. 10 mV[sum= 5189 mV] Profiles 1-500 Smooth Av 5 -Baseline 20



Shimadzu Biotech Axima Confidence 2.9.3.20110624: Mode Reflectron_neg, Power: 80, Blanked, P.Ext. @ 400 (bin 58)
%Int. 30 mV[sum= 14829 mV] Profiles 1-500 Smooth Av 5 -Baseline 20

