Supporting Information

Topological and electron transfer properties of 2-Thiobarbituric acid ad-layer on polycrystalline gold electrodes

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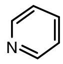
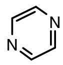
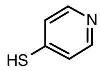
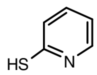
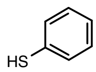
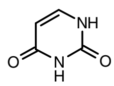
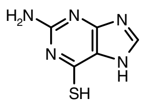
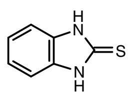
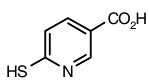
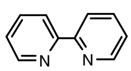
Experimental details.

The QCM cell consisted of three round Teflon pieces, 37 mm in total height and 35 mm in diameter. The top piece was the cell top to hold the reference and counter electrodes, and two 2 mm holes for manual purging; the central piece was the cell body for the solution; and the bottom piece was for mounting purpose. The quartz crystal was located between the central and the bottom pieces. The seal is made through two O-rings pressed together by four screws that tighten the bottom and central pieces.

The circular-shaped gold layer of 5 mm diameter (geometric area = 0.196 cm^2) was electrically connected by a small gold flag. The exact gold surface exposed to the solution was calculated with the aid of image analysis (Rasband, W. *ImageJ*, version 1.30v; U. S. National Institute of Health: Bethesda, MD) after digitalization of the electrode. For such purpose, the scanned image included the O-rings, in order to reproduce as exactly as possible the experimental conditions. The measured area of the gold flag was 0.019 cm^2, that is, 9.7 % of the circular gold layer. As the area of this flag introduces a constant but significant error in the calculations, the corrected area (0.215 cm^2) was considered as the actual geometric area in all calculations.

Packing densities and surface coverages for different heterocyclic compounds adsorbed on gold

Compound		Packing density	Surface	Reference
Name	Structure	molec cm^{-2}	coverage[a]	
Pyridine		0.40×10^{15}	0.27	[1]
Pyrazine		0.36×10^{15}	0.24	[2]
4-mercaptopyridine		0.26×10^{15} 0.69×10^{15}	0.17 (in $HClO_4$) 0.46 (in H_2SO_4)	[3] [4]
2-mercaptopyridine		0.28×10^{15}	0.18	[3]
Thiophenol		0.28×10^{15}	0.18	[3]
Uracil		0.48×10^{15} 0.25×10^{15}	0.32 0.17	[2] [5]
6-mercaptopurine		0.34×10^{15}	0.23	[6]
2-amino-6-mercaptopurine		0.40×10^{15}	0.27	[7]
2-mercaptobenzimidazole		0.29×10^{15}	0.20	[8]
6-mercaptonicotinic acid		0.12×10^{15}	0.08	[9]
2,2’-bipyridine		0.3×10^{15}	0.20	[10]

[a] Calculated on the basis of a gold packing density of 1.5×10^{15} at cm^{-2}.

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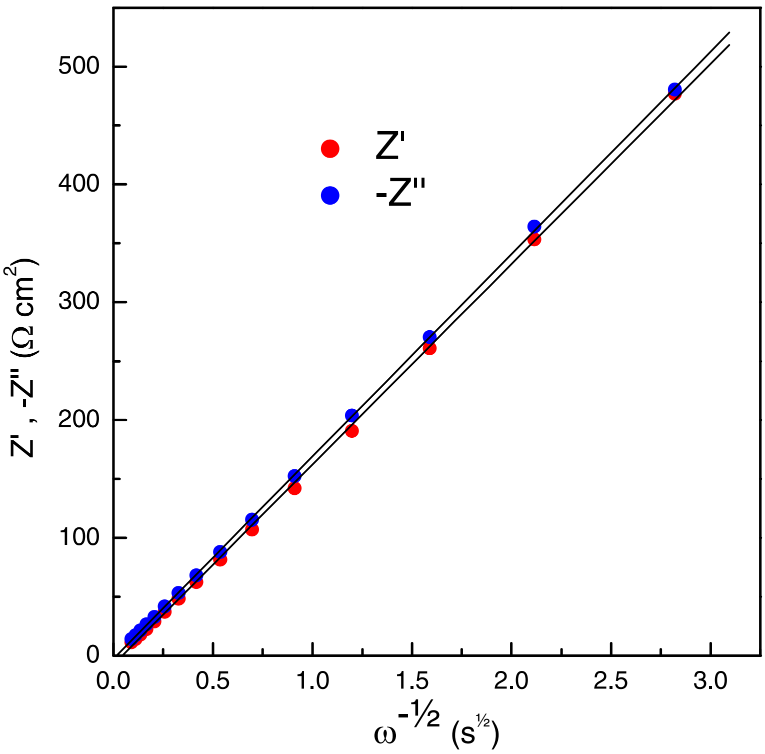
The Warburg coefficient, σ_W, can be obtained from the slopes of the plots corresponding to the imaginary (-Z'') and real (Z') parts of the total impedance vs. $\omega^{-½}$ after correction for the solution resistance. For a system under linear-diffusion control, both plots should coincide, as shown in the following graph.



The values for the slopes from the linear regressions (value ± standard deviation), along with the values for the regression coefficients are:

Z' vs. $\omega^{½}$: 171.9 ± 0.5 Ω cm^2 s$^{-½}$ (r = 0.99996)
Z' vs. $\omega^{½}$: 170 ± 1.1 Ω cm^2 s$^{-½}$ (r = 0.99974)