Supplementary Material

Synthesis and spectral comparison of electronic and molecular properties of some hydrazines and hydrazyl free radicals

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Table S1. Crystallographic data, details of data collection and structure refinement parameters for compound **5a.**

Chemical formula	$C_{18}H_{11}N_5O_6$
M (g mol^{-1})	393.32
Temperature, (K)	293(2)
Wavelength, (Å)	0.71073
Crystal system	*Monoclinic*
Space group	*P2$_1$/a*
a(Å)	10.0415(7)
b(Å)	24.5824(15)
c(Å)	14.6763(14)
α(°)	90
β(°)	107.858(6)
γ(°)	90
V(Å^3)	3448.2(5)
Z	8
D_c (g cm^{-3})	1.515
μ (mm^{-1})	0.118
F(000)	1616
Goodness-of-fit on F^2	0.998
Final *R1,wR$_2$* [$I>2\sigma(I)$]	0.0477, 0.1160
*R*1, *wR$_2$*(all data)	0.0949, 0.1364
Largest diff. peak and hole (eÅ^{-3})	0.245, -0.225

Table S2. Selected bond lengths (Å) for the compound **5a.**

C1-C2 = 1.373(3)	C19-C20 = 1.370(3)	N1-N2 = 1.378(2)
C1-N1 = 1.393(2)	C19-C24 = 1.387(3)	N2-H2N = 0.86(2)
C1-C6 = 1.397(2)	C19-N6 = 1.401(2)	N3-O1 = 1.217(2)
C2-C3 = 1.381(3)	C20-C21 = 1.375(3)	N3-O2 = 1.219(2)
C3-C4 = 1.388(3)	C21-C22 = 1.373(4)	N4-O3 = 1.209(2)
C4-C5 = 1.368(3)	C22-C23 = 1.353(4)	N4-O4 = 1.209(2)
C5-C6 = 1.392(3)	C23-C24 = 1.404(3)	N5-O5 = 1.221(3)
C6-C7 = 1.449(3)	C24-C25 = 1.438(3)	N5-O6 = 1.223(3)
C7-C8 = 1.388(3)	C25-C26 = 1.391(3)	N6-N7 = 1.377(2)
C7-C12 = 1.397(3)	C25-C30 = 1.395(3)	N7-H1N = 0.88(2)
C8-C9 = 1.373(4)	C26-C27 = 1.359(4)	N8-O8 = 1.213(2)
C9-C10 = 1.380(4)	C27-C28 = 1.370(4)	N8-O7 = 1.2214(19)
C10-C11 = 1.384(3)	C28-C29 = 1.401(4)	N9-O10 = 1.213(2)
C11-C12 = 1.382(3)	C29-C30 = 1.387(3)	N9-O9 = 1.225(2)
C12-N1 = 1.396(2)	C30-N6 = 1.389(3)	N10-O12 = 1.205(3)
C13-N2 = 1.346(3)	C31-N7 = 1.353(2)	N10-O11 = 1.230(3)
C13-C18 = 1.416(3)	C31-C36 = 1.411(3)	
C13-C14 = 1.419(2)	C31-C32 = 1.421(3)	
C14-C15 = 1.375(3)	C32-C33 = 1.371(3)	
C14-N3 = 1.468(2)	C32-N8 = 1.457(2)	
C15-C16 = 1.370(3)	C33-C34 = 1.364(3)	
C16-C17 = 1.370(3)	C34-C35 = 1.376(3)	
C16-N4 = 1.450(3)	C34-N9 = 1.462(2)	
C17-C18 = 1.360(3)	C35-C36 = 1.363(3)	
C18-N5 = 1.472(3)	C36-N10 = 1.474(3)	

Table S3. Main parameters for calculation of standard rate constants of **1c-5c.**

Compound	ΔE_p (mV)	Ψ	K^o (cm/s)
1c	90	0.75	0.182
2c	150	0.25	0.061
3c	90	0.75	0.182
4c	90	0.75	0.182
5c	80	1	0.242

Figure S1. IR spectrum of the new compound **4a.**

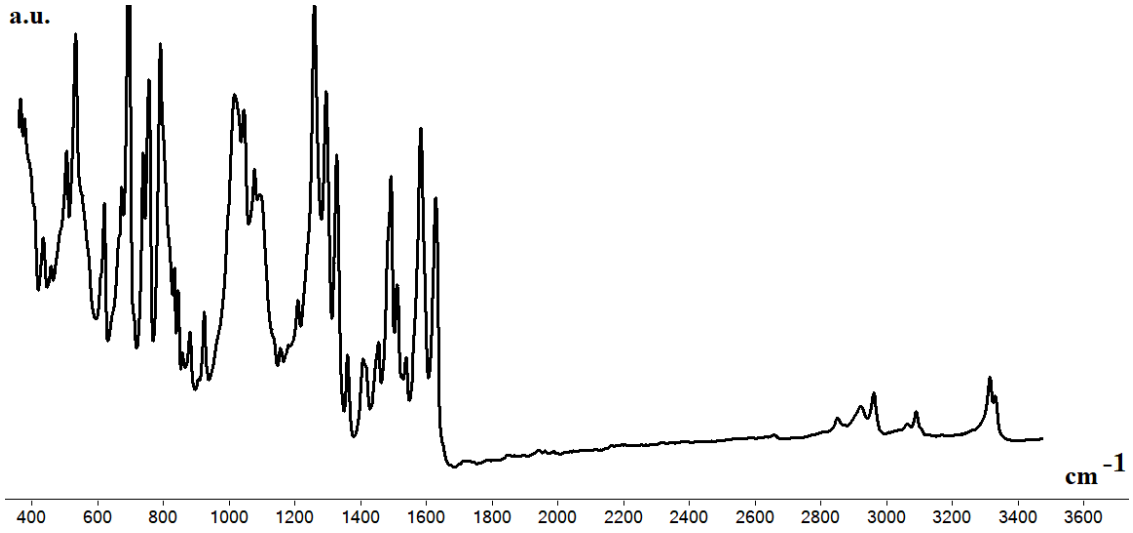


Figure S2. ^{1}H-NMR of the new compound **4a.**

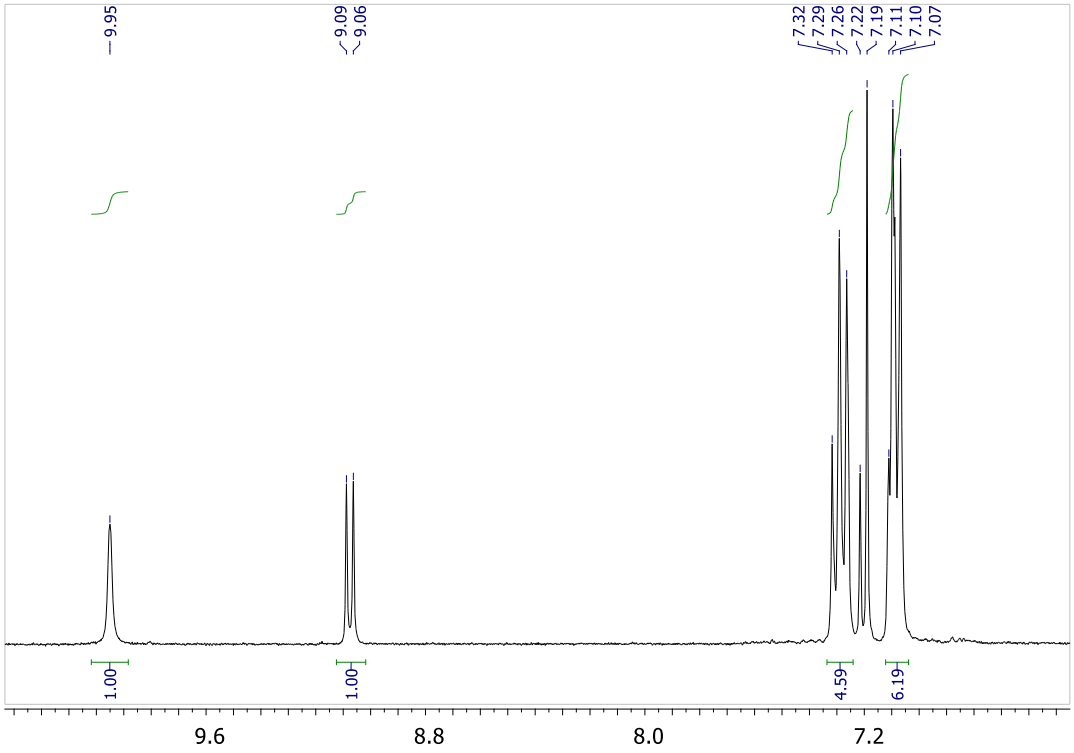


Figure S3. ^{13}C-NMR of the new compound **4a.**

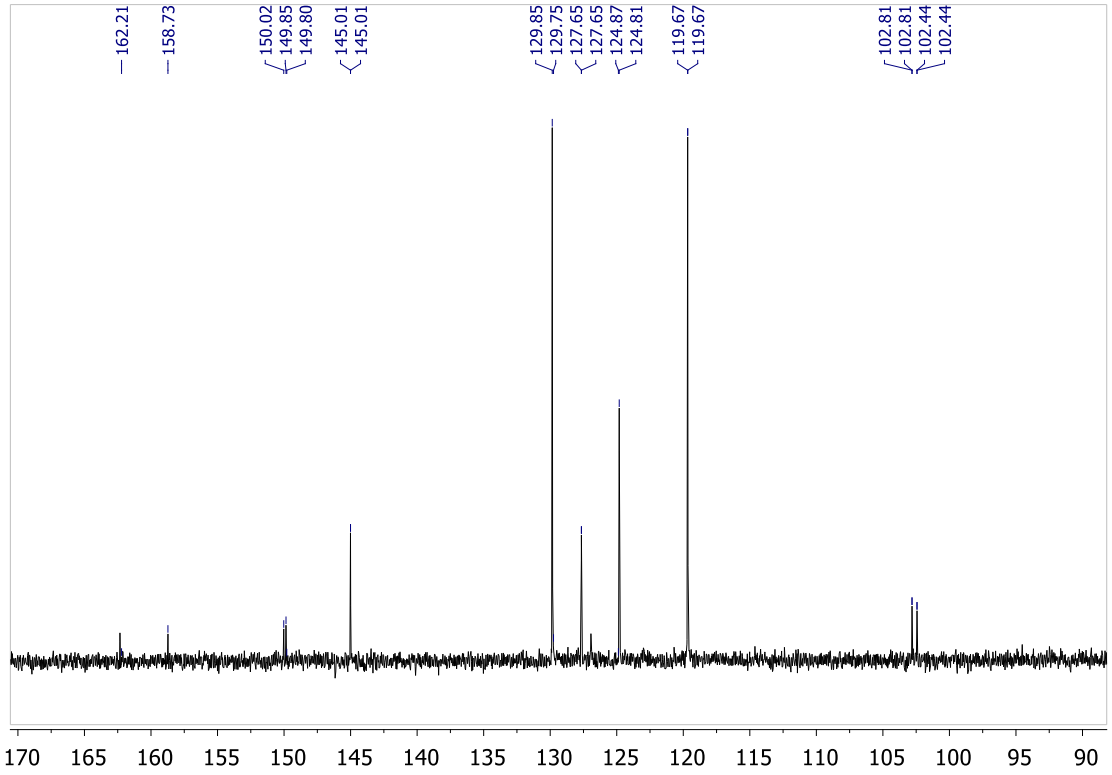


Figure S4. UV-Vis spectra of the hydrazines **1a-5a** (blue) and their anions **1c-5c** (red.)

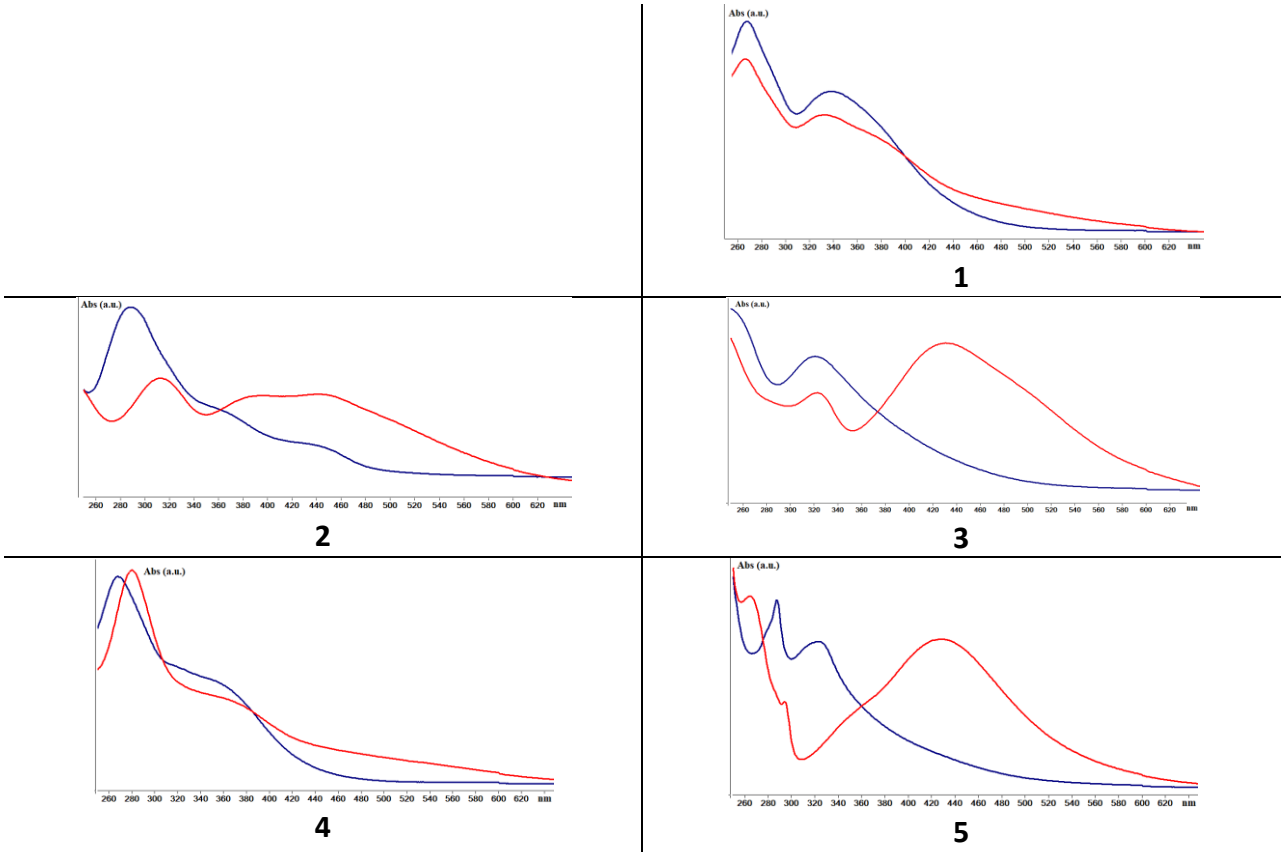


Figure S5. UV-Vis spectra of the free radicals **1b-5b.**

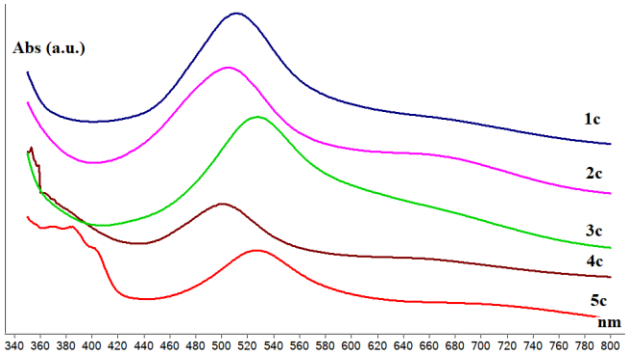
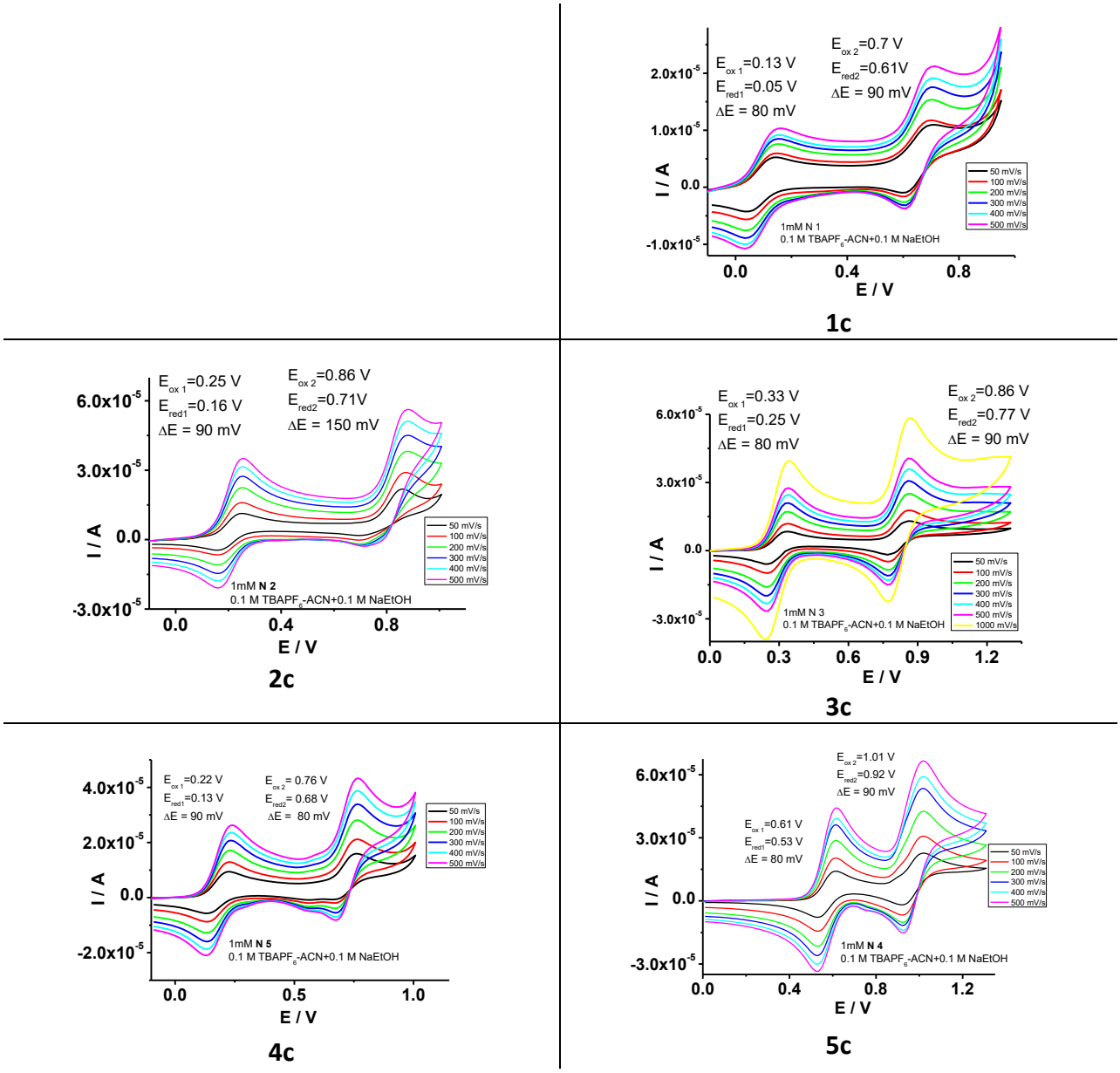


Figure S6. Cyclic voltammetry of the anions **1c-5c.**



1c **2c** **3c** **4c** **5c**