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Supplementary Info

Phosphorus-Nitrogen Compounds. Part 35. Syntheses, Spectroscopic and Electrochemical Properties, Antituberculosis, Antimicrobial and Cytotoxic Activities of Mono-Ferrocenyl-SpiroCyclotetraphosphazenes

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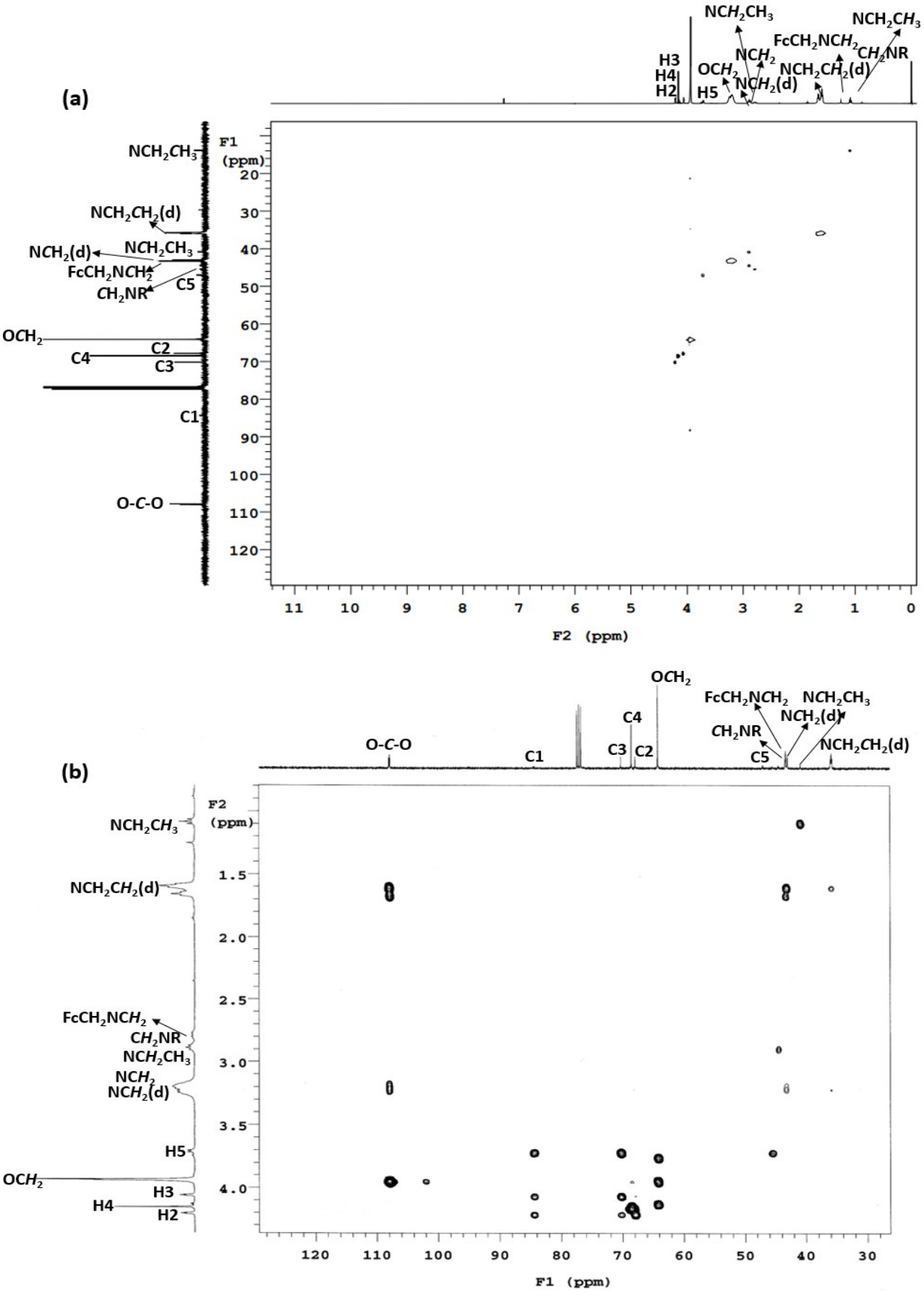

Fig. S1 The (a) HSQC and (b) HMBC spectra of **5c**.

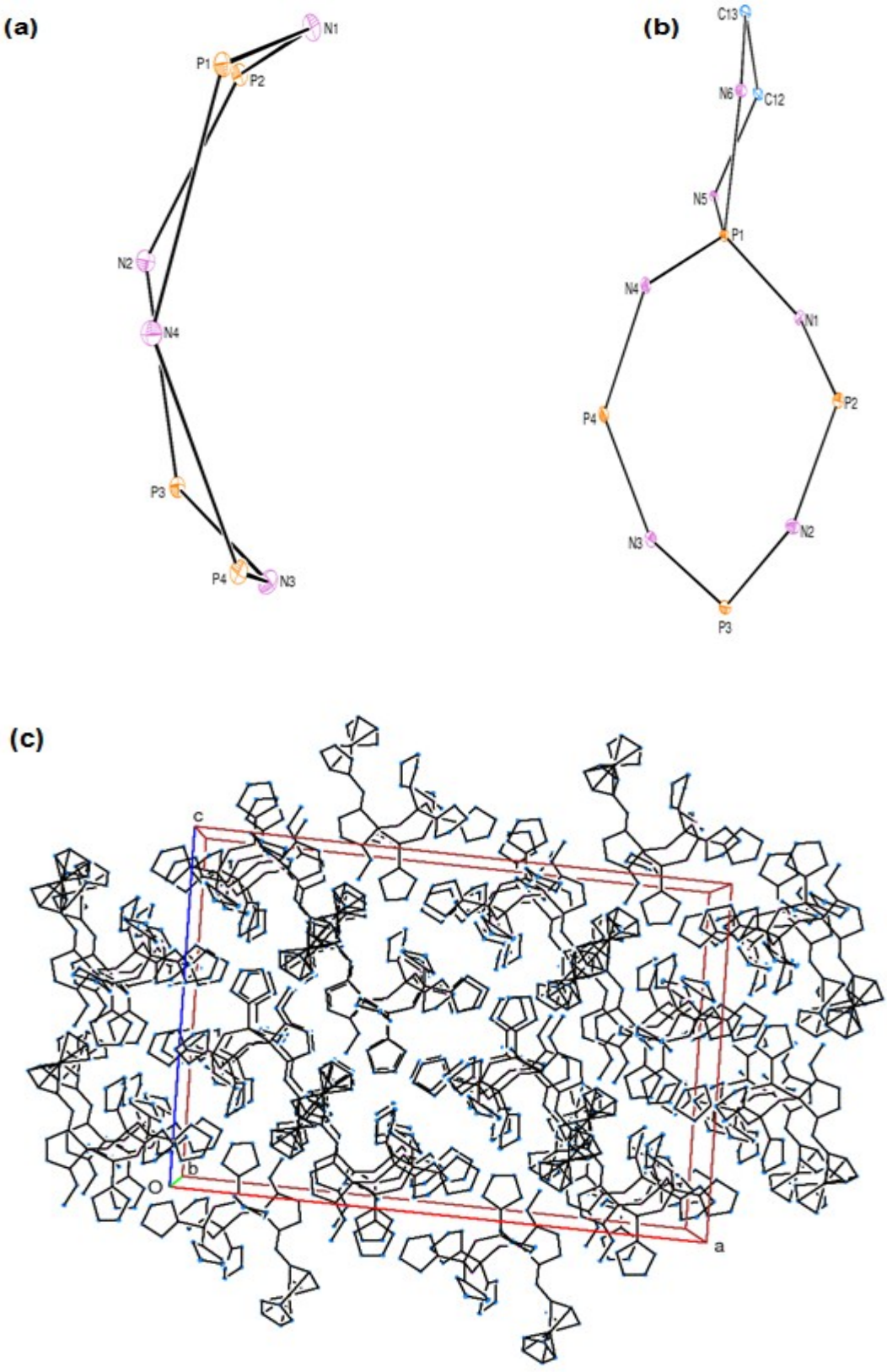

Fig. S2 The conformations of (a) the tetrameric phosphazene rings and (b) the six-membered spiro-rings (c) the packing diagram of **4a**.

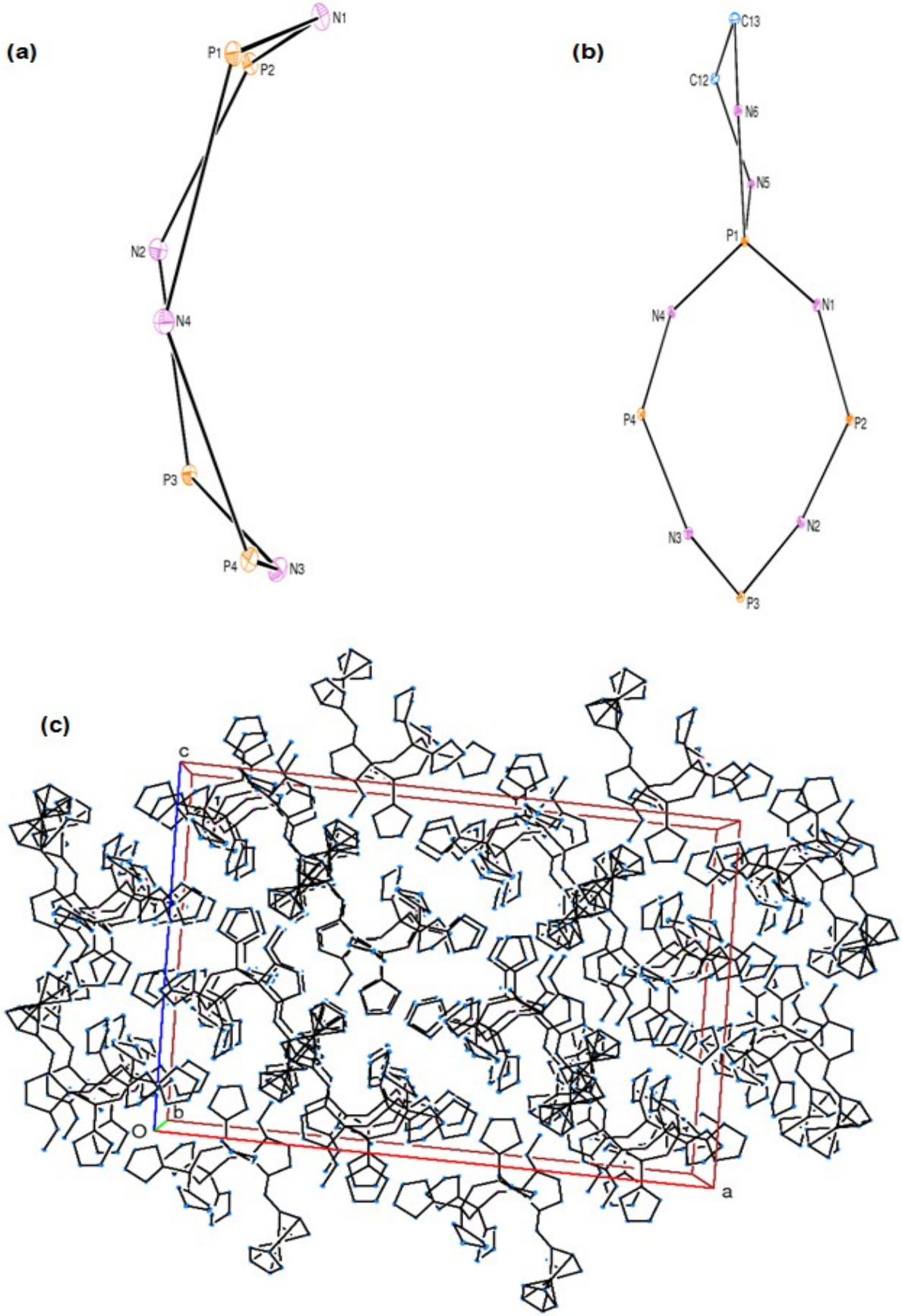

Fig. S3 The conformations of (a) the tetrameric phosphazene rings and (b) the six-membered spiro-rings (c) the packing diagram of **5a**.

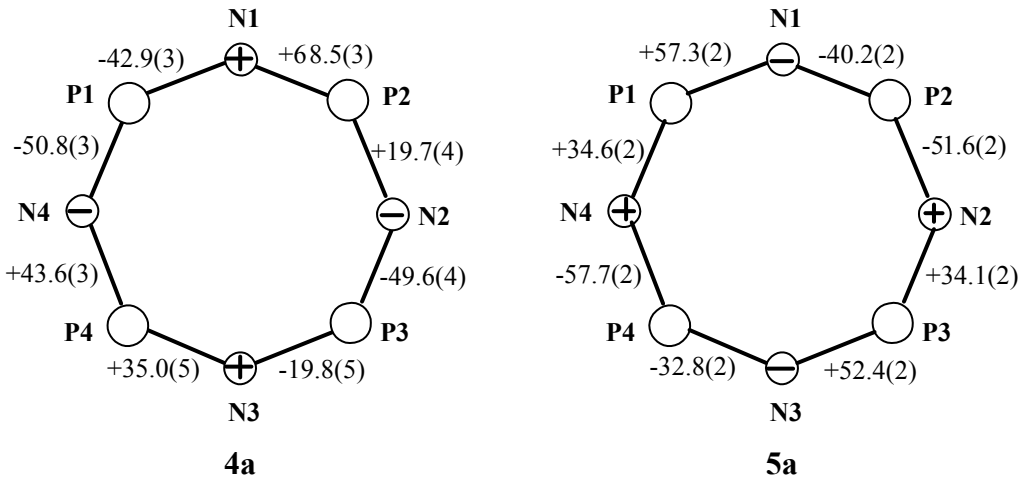

Fig. S4 The shape of the phosphazene rings in **4a** and **5a** with torsion angles (deg) given.

Table S1 CVs data of ferrocenylphosphazene derivates (1 mM each) obtained in acetonitrile (0.1 M TBATFB) at the gold electrode versus $Ag/AgNO_3$ (0.01 M). The scan rate is 100 mV s^{-1}

Compound	E_{pa}, E_{pc}, $E^{o'}$(≈ $E_{1/2}$)*	ΔEp (E_{pa}-E_{pc})	i_{pa} (μA)	i_{pc}/i_{pa}	Slope of log (i_a)-log (υ)	D cm^2 s^{-1}	Ref
4a	429, 354, 391	75	11.28	0.96	0.51	$1.77x10^{-5}$	This work
4b	515, 436, 475	79	12.74	0.96	0.52	$0.75x10^{-5}$	This work
4c	505, 422, 463	83	5.74	0.97	0.52	$0.45x10^{-5}$	This work
5a	431, 352, 391	79	12.92	0.97	0.50	$1.65x10^{-5}$	This work
5b	519, 436, 477	83	14.90	0.96	0.49	$0.87x10^{-5}$	This work
5c	491, 417, 454	74	7.86	0.96	0.51	$0.54x10^{-5}$	This work
6a	431, 353, 392	78	14.68	0.97	0.49	$1.65x10^{-5}$	This work
6b	521, 436, 478	85	18.80	0.98	0.51	$0.96x10^{-5}$	This work
6c	493, 412, 452	81	9.64	0.97	0.49	$0.67x10^{-5}$	This work
N_3P_3[$FcCH_2N(CH_2)_3NH$(pyrrolidino)$_4$]	-,-,130	76	3.88	0.93	0.51	-	**[29]**
N_3P_3[$FcCH_2N(CH_2)_2NCH_3$(pyrrolidino)$_4$]	177, 90, 134	87	18.92	1.01	0.51	$0.96×10^{-5}$	**[38]**
N_3P_3[$FcCH_2N(CH_2)_2NC_2H_5$(pyrrolidino)$_4$]	165, 94, 130	71	19.55	0.93	0.50	$0.96×10^{-5}$	**[38]**
N_3P_3[$FcCH_2N(CH_2)_2NCH_3$(vanillinato)$_4$]	210, 155, 183	55	17.91	0.95	0.53	$2.74 × 10^{-6}$	**[4]**
N_3P_3[$FcCH_2N(CH_2)_2NC_2H_5$(vanillinato)$_4$]	211, 156, 184	55	20.03	1.23	0.49	$3.08 × 10^{-6}$	**[4]**
N_3P_3[$FcCH_2N(CH_2)_3NH$(vanillinato)$_4$]	-,-,87	115	4.32	0.93	0.47	-	**[57]**
N_3P_3[$FcCH_2N(CH_2)_3NH$(morpholino)$_4$]	115, 46, 81	69	2.61	0.85	0.52	-	**[34]**
$N_4P_4Cl_2$[($FcCH_2N(CH_2)_2NCH_3$) ({$OC_6H_4CH_2$}$_2$$N(CH_2)_2$N]	509, 440, 475	69	7.74	0.95	0.46	$1.48 x 10^{-5}$	**[35]**
$N_4P_4Cl_2$[($FcCH_2N(CH_2)_2NC_2H_5$) ({$OC_6H_4CH_2$}$_2$$N(CH_2)_2$N]	509, 435, 472	74	7.08	0.94	0.48	$1.42 x 10^{-5}$	**[35]**
$N_4P_4Cl_2$[($FcCH_2N(CH_2)_3NCH_3$) ({$OC_6H_4CH_2$}$_2$$N(CH_2)_2$N]	530, 445, 530	85	7.57	1.01	0.49	$1.40 x 10^{-5}$	**[35]**
$N_4P_4Cl_2$[($FcCH_2N(CH_2)_2NCH_3$) ({$OC_6H_4CH_2$}$_2$$N(CH_2)_3$N]	514, 445, 480	69	7.11	1.02	0.52	$1.37 x 10^{-5}$	**[35]**
$N_4P_4Cl_2$[($FcCH_2N(CH_2)_2NC_2H_5$) ({$OC_6H_4CH_2$}$_2$$N(CH_2)_3$N]	521, 436, 479	85	7.60	0.95	0.53	$1.30 x 10^{-5}$	**[35]**
$N_4P_4Cl_2$[($FcCH_2N(CH_2)_3NCH_3$) ({$OC_6H_4CH_2$}$_2$$N(CH_2)_3$N]	501, 437, 469	64	7.25	0.98	0.45	$1.32 x 10^{-5}$	**[35]**

The standard deviation is 0.58 mV for peak potential measurements, 0.11 μA for peak current measurements and $0.12x10^{-5}$ cm^2 s^{-1} for diffusion coefficients.
*$E_{1/2}$ is calculated from the equation $E_{1/2} = [(E_{pa} - E_{pc})/2]+E_{pc}$ assuming reversible oxidation of Fc groups.