JOTCS A
Journal of the Turkish Chemical Society
Section: A
Chemistry
TURKISH CHEMICAL SOCIETY

The Synthesis of New Phosphazene-Bearing Ethyl p-Hydroxybenzoate and Ferrocenyl Pendant Groups and their Spectroscopic and Crystallographic Characterizations

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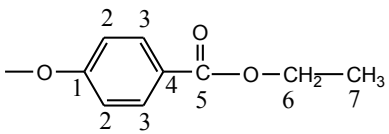
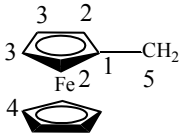
Supplementary Materials

Table S1 ^{13}C NMR (decoupled) spectral data for 2, gem-3a, *trans*[a]-3b*, trans*[b]-3c, *cis*-3d, 4 and 5 [Chemical shifts (δ) reported in ppm and *J* values in Hz].

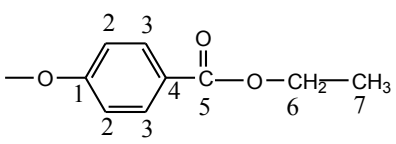


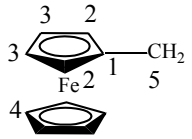


	N-CH₂-*C*H₂-	**N-*C*H₂-*C*H₂-**	**O-*C*H₂-CH₂-**	**Fc-CH₂ carbon atoms**					**Substituent carbon atoms**						
				C5	**C4**	**C3**	**C2**	**C1**	**C7**	**C6**	**C5**	**C4**	**C3**	**C2**	**C1**
2	25.77(d)	45.10	68.42(d)	47.20(d)	68.66	67.85	69.98(d)	81.90(d)	14.34	61.17	165.72	131.47	128.28(d)	121.32(d)	153.39(d)
	$^3J_{PC}$=4.5		$^2J_{PC}$=7.5	$^2J_{PC}$=3.0			$^4J_{PC}$=13.5	$^3J_{PC}$=9.8					$^4J_{PC}$=2.3	$^3J_{PC}$=5.3	$^2J_{PC}$=9.8
***gem*-3a**	25.79	44.96	68.54	46.88	68.02	67.71	69.60	82.26	14.33	61.19	165.84	131.43	127.93	121.16(d)	153.96(d)
													127.74	$^3J_{PC}$=4.5	$^2J_{PC}$=7.5
													125.53		153.69
															$^2J_{PC}$=6.0
***trans*[a]-3b. *trans*[b]-3c and *cis*-3d**	29.71	45.06	69.66	47.11	68.66	67.65	70.07	82.16	14.33	61.16	165.70	131.38	128.08	121.62	153.59
	25.85				68.57		69.90							121.56	
					68.47									121.41	
					68.37									121.34	
					68.12									121.17	
4	25.90	44.89	67.91	46.73	68.53	67.35	69.93	82.47	14.33	61.16	165.74	131.35	127.85(d)	121.52(d)	153.74(d)
					68.44	67.26	69.61	82.32		61.10		131.28	$^4J_{PC}$=1.5	$^3J_{PC}$=4.5	$^2J_{PC}$=9.8
										61.08			127.77(d)	121.12(d)	154.07(d)
													$^4J_{PC}$=1.5	$^3J_{PC}$=5.3	$^2J_{PC}$=7.5

													127.47	120.86(d)	
														$^{3}J_{PC}$=5.3	
5	25.99	44.98	68.11	46.77	68.46	67.15	69.48	82.30	14.33	61.14	165.80	131.33	127.35	120.82(dd)	154.51(dd)
										61.04	165.74	131.17	127.33	$^{3}J_{PC}$=6.0	$^{2}J_{PC}$=7.5
														120.75(dd)	154.13(dd)
														$^{3}J_{PC}$=5.3	$^{2}J_{PC}$=7.5

Table S2 ^{1}H-NMR spectral data for 2, gem-3a, *trans*[a]-3b, *trans*[b]-3c, *cis*-3d, 4 and 5. [s: singlet, d: doublet, t: triplet, m: multiplet and bp: broad peak].





	N-CH_2-$\underline{C}H_2$-	**N-$C\underline{H}_2$-CH_2-**	**O-$\underline{C}H_2$-CH_2-**	**Fc-CH_2 hydrogen atoms**				**Substituent hydrogen atoms**			
				H5	**H4**	**H3**	**H2**	**H2**	**H3**	**H6**	**H7**
2	1.92 2H	3.08 2H	4.15 2H	3.89 (m) 2H	4.14 5H	4.29 2H	4.31 2H	7.40 2H	8.10 2H	4.40 (d) 2H $^{3}J_{HH}$=7.2	1.42 (t) 3H $^{3}J_{HH}$=7.2
***trans*[a]-3b. *trans*[b]-3c and *cis*-3d**	1.88 2H	3.05 2H	4.05 2H	3.92 2H	4.14 5H	4.25 2H	4.30 2H	7.29-7.46 4H	8.05-8.15 4H	4.25-4.44 4H	1.37-1.45 6H
***trans*[a]-3b. *trans*[b]-3c. *gem*-3a and *cis*-3d**	1.88 2H	3.04 2H	4.01 2H	3.71 2H	4.13 5H	4.21 2H	4.31 2H	7.28-7.47 4H	8.03-8.17 4H	4.34-4.43 4H	1.35-1.45 6H
4	1.84 (bp) 2H	2.99 (bp) 2H	3.75 2H	3.32 2H	4.02 5H	4.07 2H	4.19 2H	7.45 2H $^{3}J_{HH}$=8.7 7.24 4H $^{3}J_{HH}$=9.3	8.14(d) 2H $^{3}J_{HH}$=9.6 9.00 4H $^{3}J_{HH}$=4.8	4.33-4.42 (m) 6H	1.35-1.44 (m) 9H
5	1.81(bp) 2H	2.98 (m) 2H	4.18 (m) 2H	3.40 (d) 2H	3.92 5H	4.03 2H	4.03 2H	7.36 (d) 4H	8.07 (d) 4H	4.382 (d) 4H	1.42 (t) 6H

$^3J_{PH}$= 8.8	$^3J_{HH}$=8.7	$^3J_{HH}$=8.7	$^3J_{HH}$=7.2	$^3J_{HH}$=7.2
	7.14 (d)	7.93 (d)	4.382 (d)	1.38 (t)
	4H	4H	4H	6H
	$^3J_{HH}$=9.0	$^3J_{HH}$=8.7	$^3J_{HH}$=7.2	$^3J_{HH}$=7.2

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, CCDC No. 1816268 for **2** and 1816269 for **5**. Copies of this information may be obtained free of charge from the Director, CCDC, 12 Union Road, Cambridge CB2 1EZ, UK (fax: +44-1223-336033; e-mail: deposit@ccdc.cam.ac.uk or www: http://www.ccdc.cam.ac.uk).

Table S3 Crystal data and structure refinement parameters for compounds **2** and **5**.

Crystal data	**2**	**5**
Empirical formula	$C_{23}H_{26}Cl_3FeN_4O_4P_3$	$C_{50}H_{53}FeN_4O_{13}P_3$
Formula weight	677.59	1066.72
Crystal system	Monoclinic	Monoclinic
Space group	$P2_1/c$	Pn
a (Å)	13.8402 (2)	11.9429 (12)
b (Å)	18.8222 (2)	31.543 (3)
c (Å)	10.7335 (3)	13.6725 (13)
β (°)	97.377 (1)	90.535 (4)
V (Å^3)	2772.97 (9)	5150.5 (9)
Z	4	4
D_c (g cm^{-3})	1.623	1.376
θ range (º)	2.2-28.1	3.0-26.4
μ (mm^{-1})	1.05	0.45
Measured refls.	29809	19462
Independent refls.	6882	14820
R_{int}	0.036	0.065
S	1.04	1.16
R1/wR2	0.049/0.122	0.071/0.158
$\Delta\rho_{max}/\Delta\rho_{min}$ (eÅ^{-3})	1.60/-1.04	0.55/-0.60

Table S4 Selected bond distances and angles for compounds **2** and **5** (Å, º)

Compound 2			
P1-O1	1.573(2)	P1-N1	1.591(2)
P1-N3	1.612(3)	P1-N4	1.632(2)
P2-N1	1.568(2)	P2-N2	1.586(3)
P3-N3	1.561(3)	P3-N2	1.576(3)
N1-P1-N3	114.99(13)	O1-P1-N4	103.76(12)
N1-P2-N2	120.15(13)	N3-P3-N2	119.33(14)
Compound 5			
N2-P2	1.581(7)	N2-P1	1.580(7)
N3-P3	1.578(7)	N3-P2	1.584(7)
N4-P3	1.573(7)	N4-P1	1.598(7)
N6-P5	1.572(7)	N6-P4	1.594(7)
N7-P5	1.573(7)	N7-P6	1.593(7)
N8-P6	1.580(7)	N8-P4	1.598(8)
N2-P1-N4	116.6(4)	O1-P1-N1	103.7(3)
N2-P2-N3	118.6(4)	N4-P3-N3	118.0(4)
N6-P4-N8	115.7(4)	O14-P4-N5	103.6(3)
N6-P5-N7	118.7(4)	N8-P6-N7	118.7(4)