Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Synthesis and characterization of a novel oxo-bridged binuclear iron(III) complex: Its catalytic application in synthesis of benzoxazoles using benzyl alcohol in water

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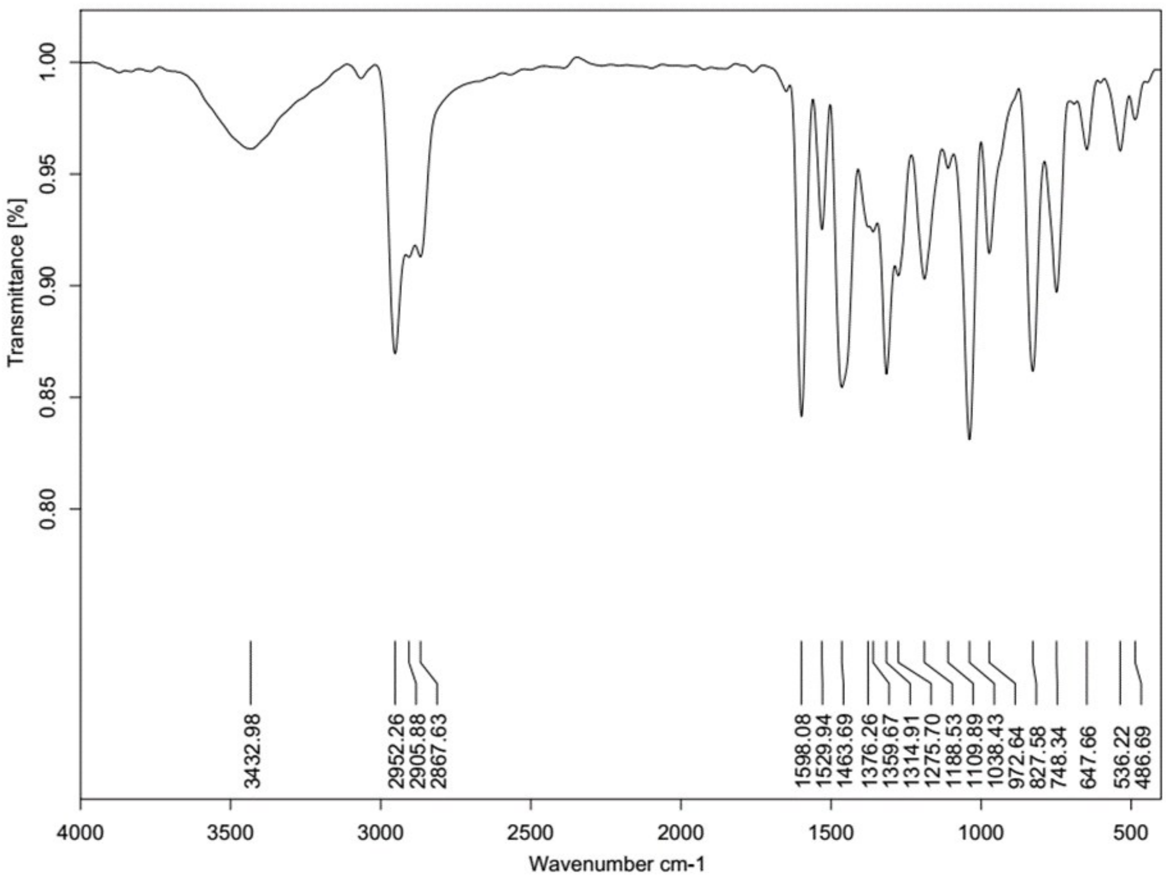
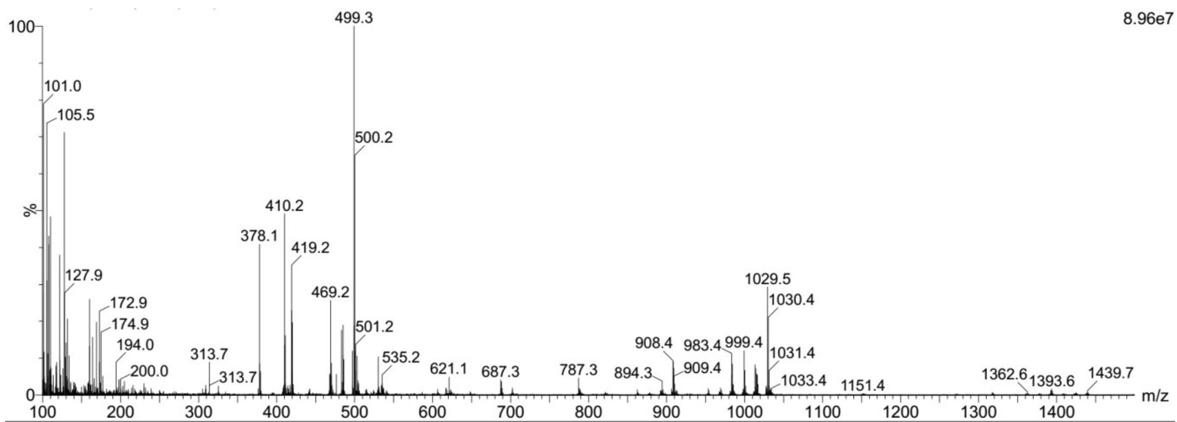
Outline

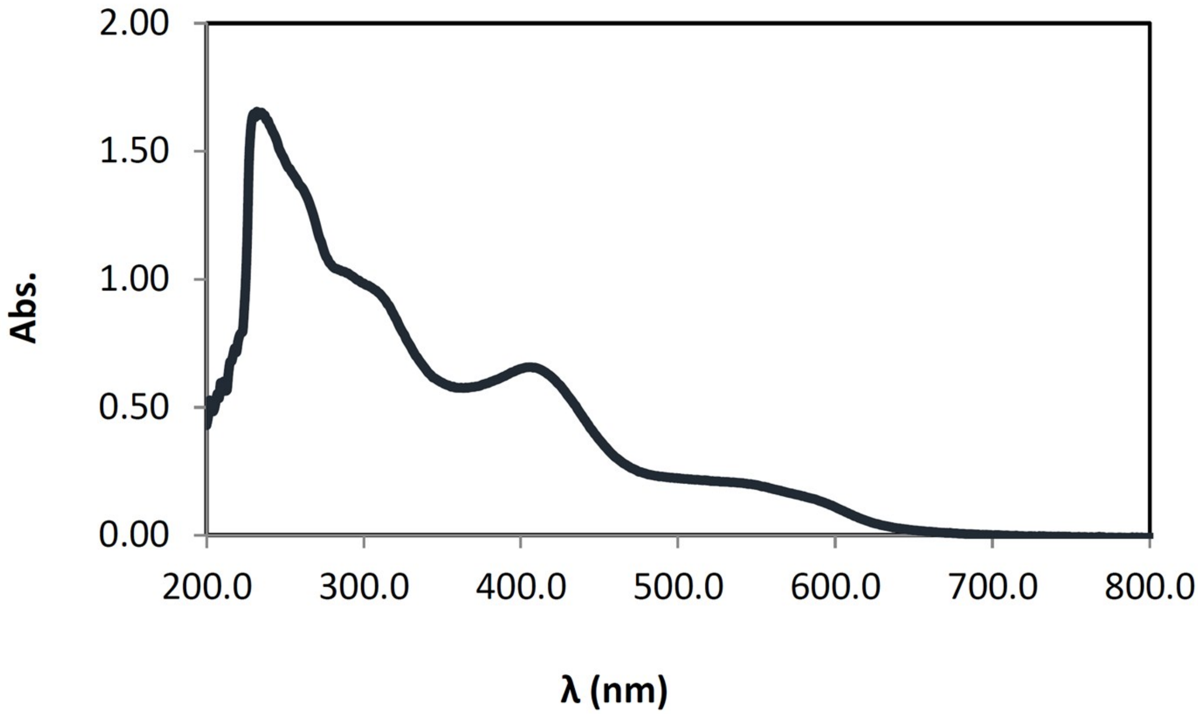
1. Figure 1S: FT-IR spectrum of $(FeL^{APIP})_2O$ complex



2. **Figure S2**. ESI-MS spectrum of $(FeL^{APIP})_2O$ complex



3. **Figure S3**. UV-Vis spectrum of $(FeLAPIP)_2O$ in CH_2CL_2



4. **Table S1**. Bond lengths [A] and angles [deg] for $(FeLAPIP)_2O$

Fe(1)-O(2)	1.7766(8)
Fe(1)-O(1)	1.9376(16)
Fe(1)-N(2)	2.0108(19)
Fe(1)-N(1)	2.0579(19)
Fe(1)-N(3)	2.110(2)
O(2)-Fe(1)#1	1.7767(8)
O(1)-C(1)	1.326(3)
C(1)-C(6)	1.406(3)
(1)-C(2)	1.408(3)
C(2)-C(3)	1.387(4)
C(2)-C(20)	1.531(4)
C(3)-C(4)	1.392(4)
C(4)-C(5)	1.388(4)
C(4)-C(24)	1.539(4)
C(5)-C(6)	1.389(3)
C(6)-N(1)	1.425(3)
N(1)-C(7)	1.279(3)
C(7)-C(8)	1.447(3)
C(8)-C(9)	1.403(4)
C(8)-C(13)	1.423(4)
C(9)-C(10)	1.367(4)
C(10)-C(11)	1.368(5)
C(11)-C(12)	1.359(4)
C(12)-C(13)	1.428(3)
C(13)-N(2)	1.372(3)
N(2)-C(14)	1.438(3)
C(14)-O(3)	1.450(3)
C(14)-C(15)	1.501(4)
C(15)-N(3)	1.337(3)
C(15)-C(16)	1.393(4)
C(16)-C(17)	1.351(5)
C(17)-C(18)	1.377(5)
C(18)-C(19)	1.382(4)
C(19)-N(3)	1.329(4)
C(20)-C(21)	1.521(4)
C(20)-C(23)	1.531(4)
C(20)-C(22)	1.535(5)
C(24)-C(27)	1.504(5)
C(24)-C(26)	1.509(6)
C(24)-C(25)	1.520(6)
O(3)-C(28)	1.453(5)
O(2)-Fe(1)-O(1)	106.87(6)
O(2)-Fe(1)-N(2)	111.50(6)
O(1)-Fe(1)-N(2)	141.56(8)
O(2)-Fe(1)-N(1)	109.54(9)
O(1)-Fe(1)-N(1)	80.57(7)
N(2)-Fe(1)-N(1)	88.76(8)
O(2)-Fe(1)-N(3)	106.82(9)
O(1)-Fe(1)-N(3)	87.44(8)
N(2)-Fe(1)-N(3)	79.57(9)
N(1)-Fe(1)-N(3)	143.59(8)
Fe(1)-O(2)-Fe(1)#1	145.64(14)
C(1)-O(1)-Fe(1)	114.44(15)
O(1)-C(1)-C(6)	118.3(2)
O(1)-C(1)-C(2)	122.4(2)
C(6)-C(1)-C(2)	119.3(2)
C(3)-C(2)-C(1)	116.7(3)
C(3)-C(2)-C(20)	123.2(2)
C(1)-C(2)-C(20)	120.1(2)
C(2)-C(3)-C(4)	125.0(2)
C(5)-C(4)-C(3)	117.3(2)
C(5)-C(4)-C(24)	121.8(3)

C(3)-C(4)-C(24)	120.8(3)
C(4)-C(5)-C(6)	119.9(3)
C(5)-C(6)-C(1)	121.8(2)
C(5)-C(6)-N(1)	125.6(2)
C(1)-C(6)-N(1)	112.58(19)
C(7)-N(1)-C(6)	124.4(2)
C(7)-N(1)-Fe(1)	125.85(16)
C(6)-N(1)-Fe(1)	109.74(14)
N(1)-C(7)-C(8)	126.1(2)
C(9)-C(8)-C(13)	119.8(2)
C(9)-C(8)-C(7)	115.2(3)
C(13)-C(8)-C(7)	124.8(2)
C(10)-C(9)-C(8)	122.3(3)
C(9)-C(10)-C(11)	118.2(3)
C(12)-C(11)-C(10)	122.2(3)
C(11)-C(12)-C(13)	121.8(3)
N(2)-C(13)-C(8)	121.8(2)
N(2)-C(13)-C(12)	122.5(2)
C(8)-C(13)-C(12)	115.7(2)
C(13)-N(2)-C(14)	117.3(2)
C(13)-N(2)-Fe(1)	126.64(15)
C(14)-N(2)-Fe(1)	115.62(18)
N(2)-C(14)-O(3)	115.5(2)
N(2)-C(14)-C(15)	110.4(2)
O(3)-C(14)-C(15)	108.5(2)
N(3)-C(15)-C(16)	119.9(3)
N(3)-C(15)-C(14)	117.3(2)
C(16)-C(15)-C(14)	122.7(3)
C(17)-C(16)-C(15)	120.1(3)
C(16)-C(17)-C(18)	119.6(3)
C(17)-C(18)-C(19)	118.3(4)
N(3)-C(19)-C(18)	121.9(3)
C(19)-N(3)-C(15)	120.1(2)
C(19)-N(3)-Fe(1)	126.2(2)
C(15)-N(3)-Fe(1)	113.67(18)
C(21)-C(20)-C(2)	109.3(2)
C(21)-C(20)-C(23)	108.0(3)
C(2)-C(20)-C(23)	111.1(3)
C(21)-C(20)-C(22)	110.4(3)
C(2)-C(20)-C(22)	109.7(2)
C(23)-C(20)-C(22)	108.3(3)
C(27)-C(24)-C(26)	110.0(5)
C(27)-C(24)-C(25)	107.3(4)
C(26)-C(24)-C(25)	107.2(4)
C(27)-C(24)-C(4)	108.7(3)
C(26)-C(24)-C(4)	112.8(3)
C(25)-C(24)-C(4)	110.8(3)
C(14)-O(3)-C(28)	114.1(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

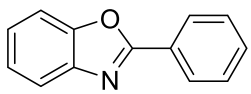
5. **Table S2**. Torsion angles [deg] for $(FeLAPIP)_2O$

O(1)-Fe(1)-O(2)-Fe(1)#1	-77.52(6)
N(2)-Fe(1)-O(2)-Fe(1)#1	104.84(7)
N(1)-Fe(1)-O(2)-Fe(1)#1	8.23(5)
N(3)-Fe(1)-O(2)-Fe(1)#1	-169.98(7)
O(2)-Fe(1)-O(1)-C(1)	89.24(17)
N(2)-Fe(1)-O(1)-C(1)	-94.30(19)
N(1)-Fe(1)-O(1)-C(1)	-18.46(15)
N(3)-Fe(1)-O(1)-C(1)	-163.95(17)
Fe(1)-O(1)-C(1)-C(6)	16.1(3)
Fe(1)-O(1)-C(1)-C(2)	-165.90(18)
O(1)-C(1)-C(2)-C(3)	-176.2(2)
C(6)-C(1)-C(2)-C(3)	1.8(3)
O(1)-C(1)-C(2)-C(20)	3.7(4)
C(6)-C(1)-C(2)-C(20)	-178.3(2)
C(1)-C(2)-C(3)-C(4)	0.0(4)
C(20)-C(2)-C(3)-C(4)	-179.9(3)
C(2)-C(3)-C(4)-C(5)	-2.1(4)
C(2)-C(3)-C(4)-C(24)	177.3(3)
C(3)-C(4)-C(5)-C(6)	2.3(4)
C(24)-C(4)-C(5)-C(6)	-177.0(2)
C(4)-C(5)-C(6)-C(1)	-0.5(4)
C(4)-C(5)-C(6)-N(1)	175.8(2)
O(1)-C(1)-C(6)-C(5)	176.5(2)
C(2)-C(1)-C(6)-C(5)	-1.6(3)
O(1)-C(1)-C(6)-N(1)	-0.3(3)
C(2)-C(1)-C(6)-N(1)	-178.4(2)
C(5)-C(6)-N(1)-C(7)	-10.2(3)
C(1)-C(6)-N(1)-C(7)	166.4(2)
C(5)-C(6)-N(1)-Fe(1)	169.2(2)
C(1)-C(6)-N(1)-Fe(1)	-14.2(2)
O(2)-Fe(1)-N(1)-C(7)	92.24(19)
O(1)-Fe(1)-N(1)-C(7)	-163.1(2)
N(2)-Fe(1)-N(1)-C(7)	-20.18(19)
N(3)-Fe(1)-N(1)-C(7)	-90.6(2)
O(2)-Fe(1)-N(1)-C(6)	-87.13(13)
O(1)-Fe(1)-N(1)-C(6)	17.54(14)
N(2)-Fe(1)-N(1)-C(6)	160.45(14)
N(3)-Fe(1)-N(1)-C(6)	89.99(18)
C(6)-N(1)-C(7)-C(8)	-173.4(2)
Fe(1)-N(1)-C(7)-C(8)	7.3(3)
N(1)-C(7)-C(8)-C(9)	-175.7(2)
N(1)-C(7)-C(8)-C(13)	9.7(4)
C(13)-C(8)-C(9)-C(10)	-1.2(4)
C(7)-C(8)-C(9)-C(10)	-176.1(3)
C(8)-C(9)-C(10)-C(11)	0.8(5)
C(9)-C(10)-C(11)-C(12)	-0.6(5)
C(10)-C(11)-C(12)-C(13)	0.8(5)
C(9)-C(8)-C(13)-N(2)	-177.9(2)
C(7)-C(8)-C(13)-N(2)	-3.5(4)
C(9)-C(8)-C(13)-C(12)	1.4(3)
C(7)-C(8)-C(13)-C(12)	175.7(2)
C(11)-C(12)-C(13)-N(2)	178.1(3)
C(11)-C(12)-C(13)-C(8)	-1.2(4)
C(8)-C(13)-N(2)-C(14)	168.4(2)
C(12)-C(13)-N(2)-C(14)	-10.8(3)
C(8)-C(13)-N(2)-Fe(1)	-19.2(3)
C(12)-C(13)-N(2)-Fe(1)	161.60(19)
O(2)-Fe(1)-N(2)-C(13)	-84.5(2)
O(1)-Fe(1)-N(2)-C(13)	99.2(2)
N(1)-Fe(1)-N(2)-C(13)	26.1(2)
N(3)-Fe(1)-N(2)-C(13)	171.4(2)

O(2)-Fe(1)-N(2)-C(14)	88.06(19)
O(1)-Fe(1)-N(2)-C(14)	-88.3(2)
N(1)-Fe(1)-N(2)-C(14)	-161.39(18)
N(3)-Fe(1)-N(2)-C(14)	-16.05(18)
C(13)-N(2)-C(14)-O(3)	70.4(3)
Fe(1)-N(2)-C(14)-O(3)	-102.9(2)
C(13)-N(2)-C(14)-C(15)	-166.0(2)
Fe(1)-N(2)-C(14)-C(15)	20.7(3)
N(2)-C(14)-C(15)-N(3)	-14.0(3)
O(3)-C(14)-C(15)-N(3)	113.5(3)
N(2)-C(14)-C(15)-C(16)	168.6(3)
O(3)-C(14)-C(15)-C(16)	-63.9(3)
N(3)-C(15)-C(16)-C(17)	0.9(5)
C(14)-C(15)-C(16)-C(17)	178.3(3)
C(15)-C(16)-C(17)-C(18)	-0.6(5)
C(16)-C(17)-C(18)-C(19)	0.7(6)
C(17)-C(18)-C(19)-N(3)	-1.2(6)
C(18)-C(19)-N(3)-C(15)	1.5(5)
C(18)-C(19)-N(3)-Fe(1)	-178.6(3)
C(16)-C(15)-N(3)-C(19)	-1.4(4)
C(14)-C(15)-N(3)-C(19)	-178.9(3)
C(16)-C(15)-N(3)-Fe(1)	178.8(2)
C(14)-C(15)-N(3)-Fe(1)	1.3(3)
O(2)-Fe(1)-N(3)-C(19)	78.6(3)
O(1)-Fe(1)-N(3)-C(19)	-28.3(3)
N(2)-Fe(1)-N(3)-C(19)	-171.9(3)
N(1)-Fe(1)-N(3)-C(19)	-98.6(3)
O(2)-Fe(1)-N(3)-C(15)	-101.58(18)
O(1)-Fe(1)-N(3)-C(15)	151.56(19)
N(2)-Fe(1)-N(3)-C(15)	7.91(19)
N(1)-Fe(1)-N(3)-C(15)	81.3(2)
C(3)-C(2)-C(20)-C(21)	115.9(3)
C(1)-C(2)-C(20)-C(21)	-63.9(3)
C(3)-C(2)-C(20)-C(23)	-3.2(4)
C(1)-C(2)-C(20)-C(23)	177.0(3)
C(3)-C(2)-C(20)-C(22)	-122.8(3)
C(1)-C(2)-C(20)-C(22)	57.3(3)
C(5)-C(4)-C(24)-C(27)	-110.0(5)
C(3)-C(4)-C(24)-C(27)	70.7(5)
C(5)-C(4)-C(24)-C(26)	12.2(5)
C(3)-C(4)-C(24)-C(26)	-167.1(4)
C(5)-C(4)-C(24)-C(25)	132.4(4)
C(3)-C(4)-C(24)-C(25)	-46.9(5)
N(2)-C(14)-O(3)-C(28)	54.9(4)
C(15)-C(14)-O(3)-C(28)	-69.6(3)

6. Spectral data for selected synthesized benzoxazoles

6.1. 2-Phenyl-1,3-benzoxazole (3a)



3a

Yield 85%, white crystals, mp: 101-102 °C [lit: 100-101 °C].[1]

^{1}H-NMR (250 MHz, $CDCl_3$/TMS) δ (ppm): 7.19-7.22 (m, 2H), 7.36-7.41 (m, 4H), 7.61-7.65 (m, 1H), 8.11-8.15 (m, 2H).

^{13}C-NMR (62.9 MHz, $CDCl_3$/TMS) δ (ppm): 110.6, 120.0, 124.6, 125.1, 127.1, 127.6, 128.9, 131.5, 142.1, 150.7, 163.0.

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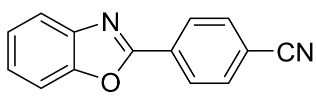
6.2. 4-(benzo[d]oxazol-2-yl)benzonitrile (3b)



3b

Yield 90%, white solid, mp: 131-132 °C [lit: 130-132 °C].[2]

^{1}H NMR (250 MHz, CDCl3): δ (ppm) = 6.90-7.05 (m, 2H), 7.25 (t,*J*= 15 Hz, 1H), 7.355 (t, *J*= 17.5 Hz, 1H), 7.77 (d, *J*= 10 Hz, 2H), 8.015 (d, *J*= 7.5 Hz, 2H).

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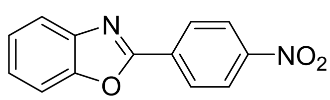
6.3. 2-(4-nitrophenyl)benzo[d]oxazole (3c)



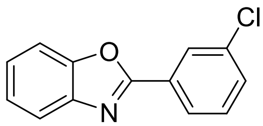
3c

Yield 91%, white solid, mp: 266.5 °C [lit: 265-267 °C].[3]

^{1}H NMR (250 MHz, CDCl3): δ (ppm) =7.35 (t, *J*= 2.5 Hz, 1H), 7.375 (t, *J*= 2.5 Hz, 2H), 7.405 (t, *J*= 2.5Hz, 1H), 7.51-7.52 (m, 2H), 7.54 (t, *J*= 5 Hz, 2H).

^{13}C-NMR (62.9 MHz, DMSO-d_6) δ (ppm): 115.1, 115.3, 120.2, 123.9, 129.0, 130.3, 134.4, 141.0, 149.0, 152.8, 152.4.

6.4. 2-(3-Chlorophenyl)benzo[d]oxazole (3d)



3d

Yield 85%, white solid, mp: 129-130 °C [lit: 130-131 °C].[4]

^{1}H-NMR (250 MHz, $CDCl_3$/TMS) δ (ppm): 7.35-7.41 (m, 2H), 7.44-7.52 (m, 2H), 7.54-7.61 (m, 1H), 7.74-7.79 (m, 1H), 8.12 (dd, *J* = 7.1, 1.6 Hz, 1H), 8.24 (d, *J* = 1.8 Hz, 1H).

^{13}C-NMR (62.9 MHz, $CDCl_3$/TMS) δ (ppm): 110.7, 120.2, 124.8, 125.5, 127.6, 128.8, 130.2, 131.5, 135.0, 141.9, 150.5, 151.2, 162.4.

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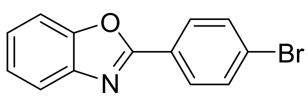
6.5. 2-(4-Bromophenyl)-1,3-benzoxazole (3e)



3e

Yield 83%, white solid, mp: 155-157 °C, [Lit: 157-158 °C].[5]

^{1}H-NMR (250 MHz, $CDCl_3$/TMS) δ (ppm): 7.29-7.36 (m, 2H), 7.48-7.55 (m, 1H), 7.60 (d, *J* = 8.55 Hz, 2H), 7.70-7.77 (m, 1H), 8.1 (d, *J* = 8.55 Hz, 2H).

^{13}C-NMR (62.9 MHz, $CDCl_3$/TMS) δ (ppm): 110.6, 120.1, 124.7, 125.3, 126.0, 126.2, 128.9, 132.2, 141.9, 150.7, 162.0.

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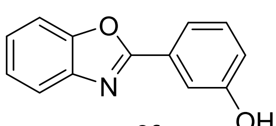
6.6. 3-(1,3-Benzoxazol-2-yl)phenol (3f)



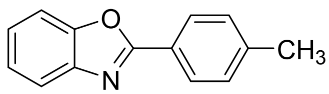
3f

Yield 80%, white solid; mp: 236-238 °C, [lit: 237-238 °C].[4]

^{1}H-NMR (250 MHz, DMSO-d_6/TMS) δ (ppm): 7.01 (dd, *J* = 7.3, 1.2 Hz, 1H), 7.30-7.40 (m, 3H), 7.60 (d, *J* = 5.8 Hz, 2H), 7.67-7.76 (m, 2H).

^{13}C-NMR (62.9 MHz, DMSO-d_6/TMS) δ (ppm): 110.7, 113.6, 118.0, 119.0, 119.6, 124.7, 125.3, 127.4, 130.3, 141.4, 150.1, 157.8, 162.3.

6.7. 2-(*p*-tolyl)benzo[d]oxazole (3g)



3g

Yield 82%, white solid, mp: 112-113 °C [Lit: 113-114 °C].[6]

^{1}H-NMR (250 MHz, DMSO-d_6/TMS) δ (ppm): 2.29 (s, 3H), 7.10-7.25 (m, 4H), 7.42-7.45 (m. 1H), 7.63-7.67 (m, 1H), 8.02 (d, *J* = 8.1 Hz, 2H).

^{13}C-NMR (62.9 MHz, DMSO-d_6/TMS) δ (ppm): 29.7, 110.5, 119.8, 124.4, 124.8, 127.6, 129.6, 142.0, 142.2, 150.6, 163.2.

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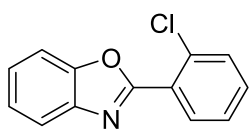
6.8. 2-(2-Chlorophenyl)-1,3-benzoxazole (3h)



3h

Yield 80%, white solid, mp: 65-66 °C; [Lit: 65-67 °C].[7]

^{1}H-NMR (250 MHz, $CDCl_3$/TMS) δ (ppm): 7.13-7.23 (m, 4H), 7.30-7.41 (m, 2H), 7.64-7.71 (m, 1H), 7.92-7.99 (m, 1H).

^{13}C-NMR (62.9 MHz, $CDCl_3$/TMS) δ (ppm): 110.7, 120.4, 124.6, 125.5, 126.1, 126.8, 131.3, 131.5, 131.7, 133.4, 141.7, 150.5, 160.8.

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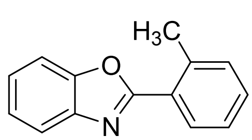
6.9. 2-(2-Methylphenyl)-1,3-benzoxazole (3i)



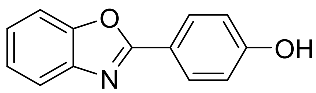
3i

Yield 86%, white solid, mp: 80-81 °C, [Lit: 80-82 °C].[4]

^{1}H-NMR (250 MHz, $CDCl_3$/TMS) δ (ppm): 2.65 (s, 3H), 7.12-7.18 (m, 5H), 7.37-7.42 (m, 1H), 7.61-7.67 (m, 1H), 7.99-8.03 (m, 1H).

^{13}C-NMR (62.9 MHz, $CDCl_3$/TMS) δ (ppm): 22.3, 110.5, 120.2, 124.4, 125.0, 126.2, 129.9, 130.9, 131.8, 138.9, 142.2, 150.3, 163.4.

6.10. 4-(Benzo[d]oxazol-2-yl)phenol (3j)



3j

Yield 78%, white solid; mp: 258-259 °C, [Lit: 259-260 °C].[4]

^{1}H-NMR (250 MHz, DMSO-d_6/TMS) δ (ppm): 6.97 (d, *J* = 8.7 Hz, 2H), 7.27-7.33 (m, 2H), 7.61-7.72 (m, 2H), 8.01 (d, *J* = 8.7 Hz, 2H), 10.35 (s, 1H).

^{13}C-NMR (62.9 MHz, DMSO-d_6/TMS) δ (ppm): 115.3, 121.3, 122.4, 124.5, 129.8, 134.0, 134.5, 147.0, 155.2, 166.1, 168.0.

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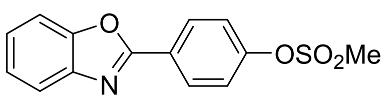
6.11. 4-(Benzo[d]oxazol-2-yl)phenyl methanesulfonate



3k

Yield 80%, white solid, mp: 167-168 °C, [Lit: 167-169 °C].[4]

^{1}H-NMR (250 MHz, $CDCl_3$/TMS) δ (ppm): 3.12 (s, 3H), 7.27 (dd, *J* = 5.8, 3.0 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.49 (dd, *J* = 5.6, 3.5 Hz, 1H), 7.68 (dd, *J* = 5.6, 3.4 Hz, 1H), 8.21 (d, *J* = 8.4 Hz, 2H).

^{13}C-NMR (62.9 MHz, $CDCl_3$/TMS) δ (ppm): 37.7, 110.7, 120.1, 122.6, 124.8, 125.5, 126.3, 129.4, 130.1, 141.8, 150.8, 151.3, 161.6.

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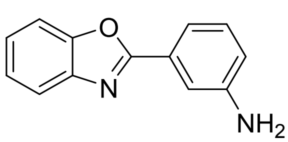
6.12. 3-(Benzo[d]oxazol-2-yl)aniline



Yield 74%, white solid, mp: 176-178 °C, [Lit: 176-177 °C].[4]

^{1}H-NMR (250 MHz, $CDCl_3$/TMS) δ (ppm): 5.48 (s, 2H), 6.79 (d, *J* = 7.6 Hz, 1H), 7.22 (t, *J* = 7.7 Hz, 1H), 7.32-7.37 (m, 3H), 7.46 (s, 1H), 7.70-7.76 (m, 2H).

^{13}C-NMR (62.9 MHz, $CDCl_3$/TMS) δ (ppm): 110.5, 113.7, 117.8, 118.2, 119.9, 124.5, 125.0, 127.9, 129.9, 142.0, 146.9, 150.7, 162.6.

7. References

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