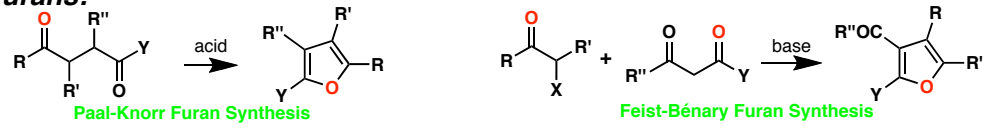
Essentials of Heterocyclic Chemistry-II

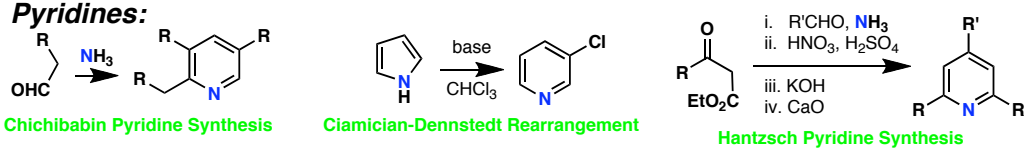
Furans:



Paal-Knorr Furan Synthesis

Feist-Bénary Furan Synthesis

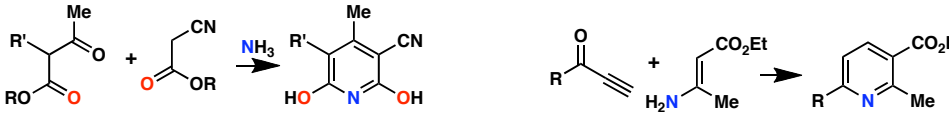
Pyridines:



Chichibabin Pyridine Synthesis

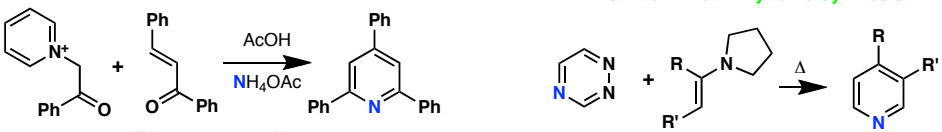
Ciamician-Dennstedt Rearrangement

Hantzsch Pyridine Synthesis



Guareschi-Thorpe Pyridine Synthesis

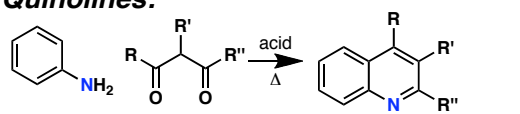
Bohlmann-Rahtz Pyridine Synthesis



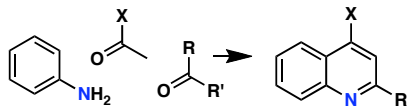
Kröhnke Pyridine Synthesis

Boger Pyridine Synthesis

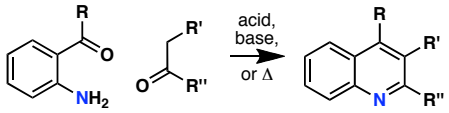
Quinolines:



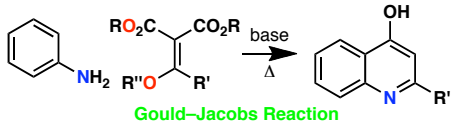
R = H/alkyl/aryl, R'' = H/alkyl/aryl Combes Quinoline Synthesis
R = O-alky/aryl, R'' = H/alkyl/aryl Conrad–Limpach Reaction
R = H/alkyl/aryl, R'' = O-alkyl Knorr Quinoline Synthesis



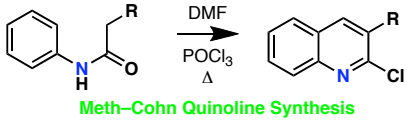
R' = H, X = CO_2H Doebner Quinoline Synthesis
R' = X = Me Riehm Quinoline Synthesis



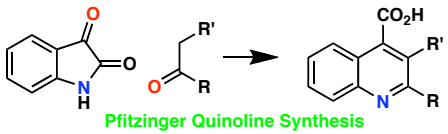
Friedländer Quinoline Synthesis



Gould–Jacobs Reaction

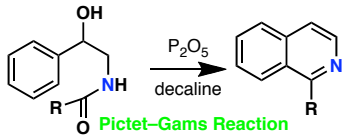


Meth–Cohn Quinoline Synthesis

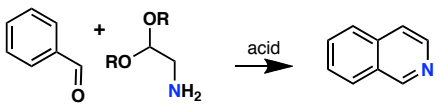


Pfitzinger Quinoline Synthesis

Isoquinolines:

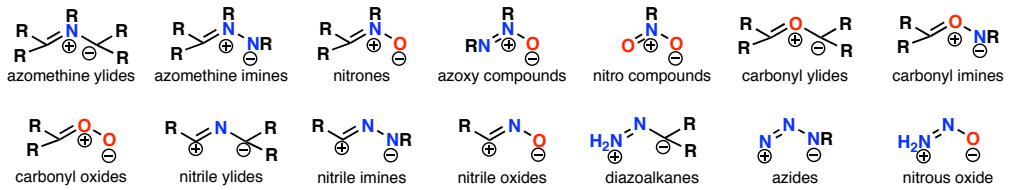


Pictet–Gams Reaction

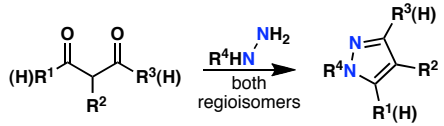


Pomeranz-Fritsch Reaction

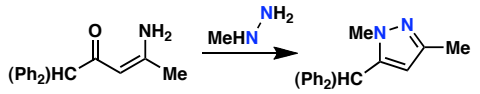
Useful 1,3-dipoles:



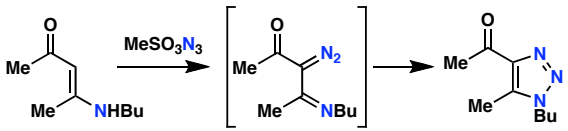
Diazoles:

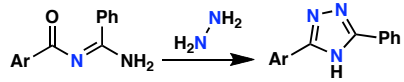


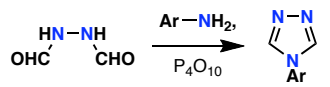
Knorr Pyrazole Synthesis

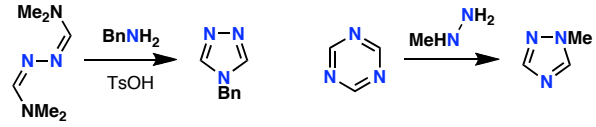


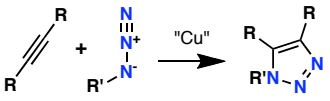
Triazoles:





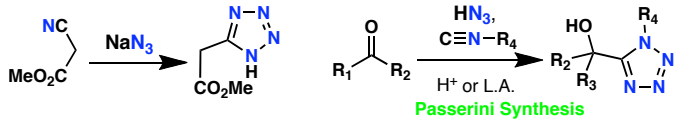






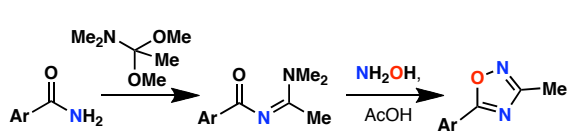
Sharpless "Click" Chemistry

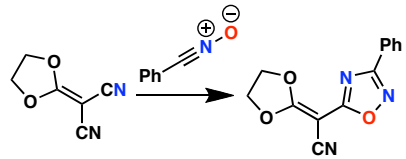
Tetrazoles:

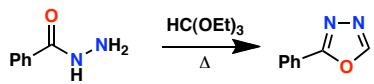


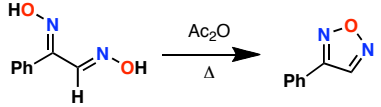
Passerini Synthesis

Oxadiazoles:

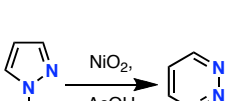


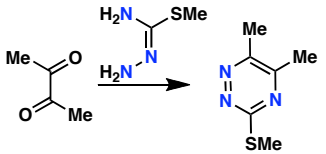


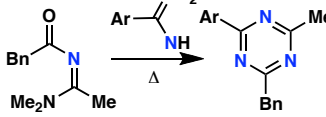




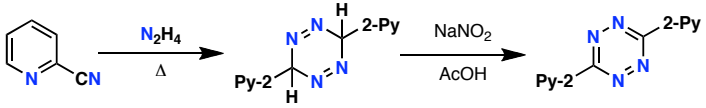
Triazanes:

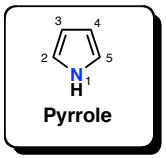






1,2,4,5-Tetrazines:



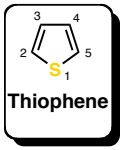


NMR Spectral Parameters

^{1}H ($CDCl_3$) ppm
H-3, H-4: 6.22
H-2, H-5: 6.68
^{13}C ($CDCl_3$)
C-3, C-4: 109.2
C-2,C-5: 117.3
H-H Coupling Constants (Hz)
$J_{2,3}$ 2.660 $J_{3,4}$ 3.359
$J_{2,4}$ 1.491 $J_{1,2}$ 2.579
$J_{2,5}$ 1.845 $J_{1,3}$ 2.458
C-H Coupling Constants (Hz)
$J_{C2\text{-}H}$ 183.28 $J_{C3\text{-}H}$ 168.80

Structural Properties

(Determined by microwave spectra)
Bond Lengths (Å)
N-C2: 1.370 NH: 0.996
C2-C3: 1.382 C2-H: 1.076
C3-C4: 1.417 C3-H: 1.077
Bond Angles
C2-N-C5: 109.8 N-C2-H2: 121.5
N-C2-C3: 107.7 C2-C3-C4: 125.5
C2-C3-C4: 107.4

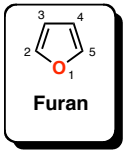


NMR Spectral Parameters

^{1}H (C_6D_{12}) ppm
H-3, H-4: 6.96
H-2, H-5: 7.20
^{13}C (acetone-d_6)
C-3, C-4: 127.3
C-2,C-5: 125.6
H-H Coupling Constants (Hz)
$J_{2,3}$ 4.9-5.8 $J_{3,4}$ 3.45-4.35
$J_{2,4}$ 1.25-1.7 $J_{2,5}$ 3.2-3.65
C-H Coupling Constants (Hz)
$J_{C2\text{-}H}$ 185 $J_{C3\text{-}H}$ 168

Structural Properties

(Determined by gas-phase microwave spectra)
Bond Lengths (Å)
S-C2: 1.714
C2-C3: 1.369
C3-C4: 1.423
Bond Angles
C2-S-C5: 92
S-C2-C3: 111
C2-C3-C4: 112

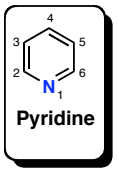


NMR Spectral Parameters

^{1}H ($CDCl_3$) ppm
H-3, H-4: 6.24
H-2, H-5: 7.29
^{13}C (acetone-d_6)
C-3, C-4: 110.4
C-2,C-5: 143.6
H-H Coupling Constants (Hz)
$J_{2,3}$ 1.75 $J_{3,4}$ 3.3
$J_{2,4}$ 0.85 $J_{2,5}$ 1.4
C-H Coupling Constants (Hz)
$J_{C2\text{-}H}$ 201 $J_{C3\text{-}H}$ 175

Structural Properties

(Determined by microwave spectra)
Bond Lengths (Å)
O-C2: 1.362
C2-C3: 1.361
C3-C4: 1.430
Bond Angles
C2-O-C5: 106.50 O-C2-H2 115.93
O-C2-C3: 110.65 C2-C3-H3 127.83
C2-C3-C4: 106.07

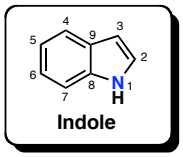


NMR Spectral Parameters

^{1}H ($CDCl_3$) ppm
H-3: 7.25
H-4: 7.64
H-2: 8.60
^{13}C ($CDCl_3$)
C-3: 123.46
C-4: 135.58
C-2 149.59
H-H Coupling Constants (Hz)
$J_{2,3}$ 4.93 $J_{2,6}$ -0.03
$J_{2,4}$ 1.80 $J_{3,5}$ 1.44
$J_{2,5}$ 1.00 $J_{3,4}$ 7.66
C-H Coupling Constants (Hz)
$J_{C2\text{-}H}$ 179 $J_{C3\text{-}H}$ 163 $J_{C4\text{-}H}$ 152

Structural Properties

(Determined by microwave and electron diffraction spectra)
Bond Lengths (Å)
N-C2: 1.338
C2-C3: 1.394
C3-C4: 1.392
Bond Angles
C6-N-C5: 116.9
N-C2-C3: 123.8
C2-C3-C4: 118.5
C3-C4-C5: 118.4

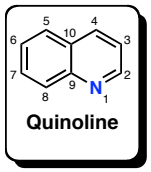


NMR Spectral Parameters

^{1}H ($CDCl_3$) ppm
H-1: 7.74 H-4: 7.64 H-7: 7.24
H-2: 7.00 H-5: 7.12
H-3: 6.51 H-6: 7.18
^{13}C ($CDCl_3$)
C-2: 124.2 C-4: 120.7 C-7: 111.1
C-3: 102.4 C-5: 119.8 C-8: 135.7
C-9: 127.8 C-6: 121.9
H-H Coupling Constants (Hz)
$J_{1,2}$ 2.5 $J_{2,3}$ 3.1 $J_{4,6}$ 1.2 $J_{5,7}$ 1.3
$J_{1,3}$ 2.0 $J_{3,7}$ 0.7 $J_{4,7}$ 0.9 $J_{6,7}$ 8.1
$J_{1,4}$ 2.8 $J_{4,5}$ 7.8 $J_{5,6}$ 7.1

Structural Properties

(x-ray of 1,3,5-trinitrobenzene complex of 3-methylindole)
Bond Lengths (Å)
N1-C2: 1.4 C4-C5: 1.37 C7-C8: 1.40
C2-C3: 1.34 C5-C6: 1.42 C8-N1: 1.38
C3-C8: 1.49 C6-C7: 1.39 C8-C9: 1.39
C8-C4: 1.37
Bond Angles
C8-N1-C2: 108 C8-C9-C4: 123 C6-C7-C8: 115
N1-C2-C3: 111 C9-C4-C5: 116 C7-C8-C9: 122
C2-C3-C9: 106 C4-C5-C6: 122 C9-C8-N1: 109
C3-C9-C8: 106 C5-C6-C7: 121

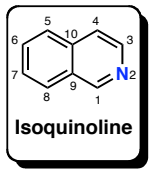


NMR Spectral Parameters

^{1}H (CCl_4) ppm
H-2: 8.82 H-5: 7.73 H-8: 8.05
H-3: 7.31 H-6: 7.46
H-4: 8.05 H-7: 7.65
^{13}C ($CDCl_3$) ppm
C-2: 150.32 C-10: 128.32 C-7: 129.40
C-3: 121.01 C-5: 127.72 C-8: 129.40
C-4: 135.93 C-6: 126.46 C-9: 148.34
H-H Coupling Constants (Hz)
$J_{2,3}$ 4.18 $J_{4,8}$ 0.75 $J_{5,8}$ 0.69 $J_{7,8}$ 8.57
$J_{2,4}$ 1.76 $J_{5,6}$ 8.24 $J_{6,7}$ 6.88
$J_{3,4}$ 8.19 $J_{5,7}$ 1.47 $J_{6,8}$ 1.25
C-H Coupling Constants (Hz)
C-2: 178 C-4: 162 C-6: 161 C-8: 161
C-3: 165 C-5: 160 C-7: 162

Structural Properties

(x-ray of NiS_2PEt_2 complex with quinoline)
Bond Lengths (Å)
N1-C2: 1.33 C10-5: 1.45 C8-C9: 1.39
C2-C3: 1.44 C5-C6: 1.35 C9-N1: 1.38
C3-C4: 1.38 C6-C7: 1.41 C9-C10: 1.43
C4-C10: 1.39 C7-C8: 1.36
Bond Angles
C9-N1-C2: 119.1 C10-C5-C6: 120.5 C10-C7-N1: 120.5
N1-C2-C3: 121.1 C5-C6-C7: 120.1 C10-C9-C8: 119.7
C2-C3-C4: 120.4 C6-C7-C8: 120.9 C4-C10-C9: 119.1
C3-C4-C10: 119.6 C7-C8-C9: 121.0 C5-C10-C9: 117.7

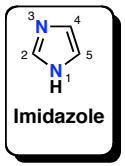


NMR Spectral Parameters

^{1}H (CCl_4) ppm
H-1: 9.11 H-5: 7.70 H-8: 7.85
H-3: 8.45 H-6: 7.56
H-4: 7.50 H-7: 7.58
^{13}C ($CDCl_3$) ppm
C-1: 152.6 C-5: 126.4 C-8: 127.5
C-3: 143.1 C-6: 130.2 C-9: 128.7
C-4: 120.4 C-7: 127.2 C-10: 135.7
H-H Coupling Constants (Hz)
$J_{1,4}$ 1.0 $J_{4,5}$ -0.36 $J_{5,8}$ 0.80 $J_{7,8}$ 8.27
$J_{3,4}$ 5.75 $J_{5,6}$ 8.29 $J_{6,7}$ 6.92
$J_{3,7}$ 0.3 $J_{5,7}$ 1.17 $J_{6,8}$ 1.21
C-H Coupling Constants (Hz)
C-1: 178 C-4: 161 C-6: 161 C-8: 161
C-3: 178 C-5: 161 C-7: 163

Structural Properties

(x-ray of C1-hydroxymethylphenyl derivative of isoquinoline)
Bond Lengths (Å)
C1-N2: 1.318 C10-5: 1.417 C8-C9: 1.414
N2-C3: 1.373 C5-C6: 1.360 C9-C1: 1.426
C3-C4: 1.349 C6-C7: 1.399 C9-C10: 1.416
C4-C10: 1.414 C7-C8: 1.364
Bond Angles
C9-C1-N2: 123.2 C4-C10-C9: 117.8
C1-N2-C3: 117.8 C4-C9-C1: 117.8
N2-C3-C4: 123.9
C3-C4-C10: 119.5



NMR Spectral Parameters

^{1}H (D_2O) ppm
H-4, H-5: 7.14
H-2: 7.73
^{13}C (D_2O) ppm
C-4, C-5: 122.3
C-2: 136.2
H-H Coupling Constants (Hz)

C-H Coupling Constants (Hz)

Structural Properties

(Determined by X-Ray)
Bond Lengths (Å)
N1-C2: 1.349
C2-N3: 1.326
N3-C4: 1.378
C4-C5: 1.358
C5-N1: 1.369
Bond Angles
C2-N1-C5: 107.2
N1-C2-N3: 111.3
C2-N3-C4: 105.4
N3-C4-C5: 109.8
C4-C5-N1: 106.3