Synthesis of some cyclooctane-based pyrazines and quinoxalines

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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H3 H 1.2360 1.2136 0.1759 0.060 Uiso 1 1 calc R . .
O4 O 0.7686(7) 0.9670(4) 0.1866(3) 0.0557(13) Uani 1 1 d . . .
N1 N 1.0788(5) 0.8187(3) 0.3888(2) 0.0225(9) Uani 1 1 d . . .
N2 N 0.7677(5) 0.9796(3) 0.4315(2) 0.0210(8) Uani 1 1 d . . .
C1 C 0.7622(6) 0.8631(4) 0.4557(2) 0.0199(9) Uani 1 1 d . . .
C2 C 0.5965(6) 0.8222(4) 0.5017(2) 0.0221(9) Uani 1 1 d . . .
H2 H 0.4919 0.8761 0.5166 0.026 Uiso 1 1 calc R . .
C3 C 0.5882(7) 0.7041(4) 0.5249(3) 0.0268(10) Uani 1 1 d . . .
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C7 C 1.0846(6) 0.9314(4) 0.3666(2) 0.0222(10) Uani 1 1 d . . .
C8 C 1.2676(6) 0.9709(5) 0.3188(3) 0.0266(10) Uani 1 1 d . . .
H8A H 1.3912 0.9217 0.3358 0.032 Uiso 1 1 calc R . .
H8B H 1.3022 1.0545 0.3330 0.032 Uiso 1 1 calc R . .
C9 C 1.2234(7) 0.9610(5) 0.2248(3) 0.0335(12) Uani 1 1 d . . .
H9A H 1.1509 0.8850 0.2116 0.040 Uiso 1 1 calc R . .
H9B H 1.3579 0.9600 0.1990 0.040 Uiso 1 1 calc R . .
C10 C 1.0862(10) 1.0663(6) 0.1884(3) 0.0490(16) Uani 1 1 d . . .
H10 H 1.0820 1.0618 0.1275 0.059 Uiso 1 1 calc R . .
C11 C 0.8640(9) 1.0560(5) 0.2137(3) 0.0426(14) Uani 1 1 d . . .
C12 C 0.7916(9) 1.1508(5) 0.2720(3) 0.0386(13) Uani 1 1 d . . .
H12A H 0.6403 1.1408 0.2781 0.046 Uiso 1 1 calc R . .
H12B H 0.8132 1.2306 0.2487 0.046 Uiso 1 1 calc R . .
C13 C 0.9128(7) 1.1421(4) 0.3570(3) 0.0241(10) Uani 1 1 d . . .
H13A H 1.0569 1.1721 0.3534 0.029 Uiso 1 1 calc R . .
H13B H 0.8437 1.1928 0.3962 0.029 Uiso 1 1 calc R . .
C14 C 0.9215(6) 1.0149(4) 0.3881(2) 0.0209(9) Uani 1 1 d . . .

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N1 0.0223(18) 0.032(2) 0.0139(16) -0.0030(15) 0.0041(13) 0.0062(15)
N2 0.0244(18) 0.0262(19) 0.0126(16) -0.0011(14) 0.0033(13) 0.0032(14)
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C3 0.031(2) 0.032(2) 0.018(2) 0.0009(18) 0.0059(17) -0.0009(19)
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C7 0.021(2) 0.036(3) 0.0101(17) -0.0035(18) 0.0033(14) 0.0018(17)
C8 0.017(2) 0.043(3) 0.020(2) -0.001(2) 0.0055(16) -0.0007(19)
C9 0.030(2) 0.053(3) 0.019(2) -0.002(2) 0.0100(17) 0.005(2)
C10 0.057(4) 0.067(4) 0.022(2) -0.002(3) 0.002(2) 0.002(3)
C11 0.044(3) 0.054(4) 0.029(3) 0.011(3) -0.001(2) -0.001(3)
C12 0.055(3) 0.039(3) 0.024(2) 0.007(2) 0.015(2) 0.019(2)
C13 0.029(2) 0.028(2) 0.018(2) -0.0036(17) 0.0117(16) 0.0009(18)
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C14 0.022(2) 0.029(2) 0.0116(18) -0.0023(17) 0.0038(14) -0.0005(17)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
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 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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N1 C6 1.380(6) . ?
N2 C14 1.321(5) . ?
N2 C1 1.371(6) . ?
C1 C2 1.427(6) . ?
C1 C6 1.431(6) . ?
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C4 C5 1.383(7) . ?
C4 H4 0.9500 . ?
C5 C6 1.415(7) . ?
C5 H5 0.9500 . ?
C7 C14 1.469(6) . ?
C7 C8 1.528(6) . ?
C8 C9 1.553(6) . ?
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C8 H8B 0.9900 . ?
C9 C10 1.567(8) . ?
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C8 C9 C10 112.3(4) . . ?
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C14 C13 H13A 109.3 . . ?
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