

Synthesis of some cyclooctane-based pyrazines and quinoxalines

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Refinement of F2 against ALL reflections. The weighted R-factor wR and
goodness of fit S are based on F2, conventional R-factors R are based
on F, with F set to zero for negative F2. The threshold expression of
F2 > 2sigma(F2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F2 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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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 . . .
H3A H 0.4789 0.6776 0.5563 0.032 Uiso 1 1 calc R . . .
C4 C 0.7423(8) 0.6222(4) 0.5019(3) 0.0307(11) Uani 1 1 d . . .
H4 H 0.7343 0.5411 0.5175 0.037 Uiso 1 1 calc R . . .
C5 C 0.9035(7) 0.6600(4) 0.4569(3) 0.0277(11) Uani 1 1 d . . .
H5 H 1.0058 0.6048 0.4420 0.033 Uiso 1 1 calc R . . .
C6 C 0.9172(6) 0.7804(4) 0.4331(2) 0.0223(10) Uani 1 1 d . . .
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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O4 0.077(3) 0.043(2) 0.042(2) 0.0111(19) -0.025(2) -0.025(2)
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)
C1 0.022(2) 0.026(2) 0.0115(17) -0.0022(16) 0.0031(14) 0.0047(17)
C2 0.022(2) 0.028(2) 0.0170(19) -0.0011(18) 0.0071(15) 0.0036(17)
C3 0.031(2) 0.032(2) 0.018(2) 0.0009(18) 0.0059(17) -0.0009(19)
C4 0.040(3) 0.025(2) 0.026(2) 0.004(2) 0.0009(19) 0.005(2)
C5 0.034(2) 0.028(2) 0.022(2) -0.0017(18) 0.0036(17) 0.0128(19)
C6 0.025(2) 0.031(2) 0.0111(18) -0.0020(17) 0.0020(15) 0.0049(18)
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)

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 and torsion angles; correlations between esds in cell parameters are only 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) . ?

C2 C3 1.384(7) . ?

C2 H2 0.9500 . ?

C3 C4 1.424(7) . ?

C3 H3A 0.9500 . ?

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) . ?

C8 H8A 0.9900 . ?

C8 H8B 0.9900 . ?

C9 C10 1.567(8) . ?

C9 H9A 0.9900 . ?

C9 H9B 0.9900 . ?

C10 C11 1.519(8) . ?

C10 H10 1.0000 . ?

C11 C12 1.529(8) . ?

C12 C13 1.550(6) . ?

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N2 C1 C6 120.8(4) . . ?
C2 C1 C6 119.2(4) . . ?
C3 C2 C1 120.1(4) . . ?
C3 C2 H2 120.0 . . ?
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C2 C3 C4 120.5(4) . . ?
C2 C3 H3A 119.8 . . ?
C4 C3 H3A 119.8 . . ?
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C4 C5 H5 119.8 . . ?
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N1 C7 C8 117.4(4) . . ?
C14 C7 C8 121.8(4) . . ?
C7 C8 C9 113.7(3) . . ?
C7 C8 H8A 108.8 . . ?
C9 C8 H8A 108.8 . . ?
C7 C8 H8B 108.8 . . ?
C9 C8 H8B 108.8 . . ?
H8A C8 H8B 107.7 . . ?
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C10 C9 H9B 109.1 . . ?
H9A C9 H9B 107.9 . . ?
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O3 C10 C9 111.1(4) . . ?
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C9 C10 H10 108.4 . . ?
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O4 C11 C12 128.6(5) . . ?
C10 C11 C12 117.0(5) . . ?
C11 C12 C13 111.5(4) . . ?
C11 C12 H12A 109.3 . . ?
C13 C12 H12A 109.3 . . ?
C11 C12 H12B 109.3 . . ?
C13 C12 H12B 109.3 . . ?
H12A C12 H12B 108.0 . . ?
C14 C13 C12 111.4(4) . . ?
C14 C13 H13A 109.3 . . ?

C12 C13 H13A 109.3 . . ?
C14 C13 H13B 109.3 . . ?
C12 C13 H13B 109.3 . . ?
H13A C13 H13B 108.0 . . ?
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C7 C14 C13 122.0(4) . . ?

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N1 C7 C14 C13 -174.3(4) ?
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C12 C13 C14 C7 86.2(5) ?

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