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submitted to *Aust. J. Chem.*

Ye-Xiang Tong

Jan. 30, 2002

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## # 2. PROCESSING SUMMARY (IUCr Office Use Only)

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\_journal\_date\_to\_coeditor ?

\_journal\_date\_from\_coeditor ?

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'x-1/2, -y-1/2, z-1/2'

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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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H1B H 0.3715 0.7225 0.1834 0.080 Uiso 1 d R . .  
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H3A H 0.4993 0.7337 0.2777 0.080 Uiso 1 d R . .  
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C4 C 0.5105(3) 0.6349(3) 0.0781(2) 0.0520(11) Uani 1 d . . .  
H4A H 0.4841 0.6568 0.0334 0.080 Uiso 1 d R . .  
H4B H 0.5266 0.5798 0.0692 0.080 Uiso 1 d R . .  
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H5A H 0.5000 0.5497 0.1937 0.080 Uiso 1 d R . .  
H5B H 0.4397 0.6064 0.2396 0.080 Uiso 1 d R . .  
C6 C 0.6333(3) 0.6461(3) 0.1680(2) 0.0583(12) Uani 1 d . . .  
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H6B H 0.6510 0.5913 0.1601 0.080 Uiso 1 d R . .  
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H7B H 0.4518 0.8770 0.1384 0.080 Uiso 1 d R . .  
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H10B H 0.3882 0.2291 0.3973 0.080 Uiso 1 d R . .  
C11 C 0.4997(3) 0.4336(3) 0.3257(2) 0.0626(13) Uani 1 d . . .



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H13B H 0.4608 0.3970 0.4930 0.080 Uiso 1 d R ..  
C14 C 0.5643(4) 0.1957(3) 0.3733(3) 0.0877(18) Uani 1 d ...  
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H14B H 0.6189 0.1995 0.3450 0.080 Uiso 1 d R ..  
H14C H 0.5819 0.1814 0.4228 0.080 Uiso 1 d R ..  
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H17B H 0.6703 -0.0110 0.0599 0.080 Uiso 1 d R ..  
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H21C H 0.8294 0.0482 0.0665 0.080 Uiso 1 d R ..  
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H22B H 0.2730 -0.0532 0.5165 0.080 Uiso 1 d R ..  
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H23B H 0.2209 0.0522 0.3516 0.080 Uiso 1 d R ..  
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H24B H 0.2471 -0.1591 0.3494 0.080 Uiso 1 d R ..  
C25 C 0.4054(3) 0.0113(2) 0.4473(2) 0.0484(10) Uani 1 d ...  
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H25B H 0.3899 0.0427 0.4892 0.080 Uiso 1 d R ..

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C17 0.0479(6) 0.0357(6) 0.0811(7) -0.0115(5) 0.0136(5) -0.0023(5)  
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N6 0.059(2) 0.047(2) 0.047(2) -0.0107(16) 0.0015(17) -0.0036(18)  
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N8 0.041(2) 0.060(2) 0.053(2) 0.0043(18) 0.0152(17) 0.0148(18)  
N9 0.0335(17) 0.0411(18) 0.0418(17) 0.0018(15) -0.0046(14) -0.0053(15)  
N10 0.041(2) 0.049(2) 0.0443(19) -0.0103(16) 0.0001(15) -0.0040(17)  
N11 0.0402(19) 0.0363(18) 0.0394(17) 0.0062(14) -0.0016(14) -0.0060(15)  
N12 0.052(2) 0.0317(18) 0.0435(18) 0.0063(15) -0.0107(15) -0.0072(16)  
N13 0.0311(17) 0.044(2) 0.0416(17) -0.0009(15) -0.0013(14) 0.0034(15)  
N14 0.040(2) 0.050(2) 0.0417(18) 0.0055(16) -0.0104(15) 0.0025(16)  
N15 0.052(2) 0.058(2) 0.0402(18) -0.0067(17) 0.0072(16) 0.0097(19)  
N16 0.0389(19) 0.047(2) 0.0453(19) 0.0046(16) -0.0033(15) 0.0028(16)  
C1 0.036(2) 0.082(4) 0.060(3) 0.009(3) 0.005(2) 0.004(2)

C2 0.051(3) 0.042(2) 0.041(2) 0.0104(18) 0.0186(19) 0.000(2)  
 C3 0.075(3) 0.051(3) 0.035(2) -0.0003(19) 0.004(2) -0.011(2)  
 C4 0.068(3) 0.056(3) 0.032(2) -0.0086(19) -0.002(2) -0.003(2)  
 C5 0.082(3) 0.042(3) 0.050(3) 0.003(2) 0.011(2) -0.018(2)  
 C6 0.043(3) 0.055(3) 0.076(3) 0.001(2) -0.013(2) 0.012(2)  
 C7 0.114(5) 0.047(3) 0.083(4) 0.004(3) 0.046(3) 0.022(3)  
 C8 0.038(2) 0.076(3) 0.040(2) -0.003(2) -0.0037(18) 0.008(2)  
 C9 0.047(2) 0.053(3) 0.044(2) -0.016(2) 0.0015(19) 0.007(2)  
 C10 0.062(3) 0.056(3) 0.075(3) 0.017(2) 0.030(3) 0.003(2)  
 C11 0.090(4) 0.041(3) 0.058(3) 0.010(2) 0.007(3) 0.007(3)  
 C12 0.048(3) 0.080(3) 0.054(3) -0.013(2) -0.008(2) 0.020(3)  
 C13 0.065(3) 0.061(3) 0.039(2) -0.005(2) 0.001(2) 0.022(3)  
 C14 0.108(5) 0.059(3) 0.098(4) 0.023(3) 0.030(3) 0.047(3)  
 C15 0.047(3) 0.052(3) 0.034(2) -0.0046(18) -0.0039(17) -0.009(2)  
 C16 0.052(3) 0.041(2) 0.038(2) 0.0052(18) 0.0012(18) -0.015(2)  
 C17 0.057(3) 0.031(2) 0.053(2) 0.0023(18) -0.001(2) -0.002(2)  
 C18 0.056(3) 0.031(2) 0.069(3) -0.005(2) -0.011(2) 0.004(2)  
 C19 0.045(2) 0.040(2) 0.040(2) 0.0049(18) -0.0111(17) -0.0123(19)  
 C20 0.041(2) 0.057(3) 0.040(2) 0.001(2) 0.0051(18) -0.011(2)  
 C21 0.041(3) 0.086(4) 0.075(3) 0.005(3) 0.001(2) 0.008(3)  
 C22 0.047(2) 0.050(3) 0.036(2) 0.0039(18) -0.0002(18) 0.001(2)  
 C23 0.043(2) 0.044(3) 0.055(3) 0.004(2) -0.003(2) 0.011(2)  
 C24 0.049(3) 0.058(3) 0.041(2) -0.011(2) -0.0079(19) 0.000(2)  
 C25 0.042(2) 0.052(3) 0.050(2) 0.003(2) -0.0084(19) -0.004(2)  
 C26 0.042(3) 0.056(3) 0.065(3) 0.004(2) 0.003(2) 0.014(2)  
 C27 0.053(3) 0.069(3) 0.038(2) 0.009(2) 0.0027(19) -0.001(2)  
 C28 0.034(2) 0.079(4) 0.089(4) 0.005(3) 0.005(2) 0.001(2)

\_geom\_special\_details

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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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loop\_

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Co1 C11 2.2613(12) . ?

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Co2 C17 2.2734(13) . ?  
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N16 C25 1.465(5) . ?  
N16 C27 1.465(5) . ?

loop\_

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C7 N1 C3 111.0(3) . . ?  
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C8 N6 C13 108.9(3) .. ?  
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C9 N7 C12 109.0(4) .. ?  
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C10 N8 C12 108.9(3) .. ?  
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