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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
 on F, with F set to zero for negative F^2^. The threshold expression of
 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
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O2 O 1.1162(4) 0.6522(3) 0.67102(19) 0.0233(7) Uani 1 1 d . . .
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C1 C 1.4610(7) 0.7635(6) 0.8615(3) 0.0243(10) Uani 1 1 d . . .
C2 C 1.3629(7) 0.6304(5) 0.8768(3) 0.0221(11) Uani 1 1 d . . .
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C2 0.020(3) 0.025(2) 0.022(2) -0.0016(19) -0.005(2) 0.003(2)
C3 0.022(3) 0.026(3) 0.026(3) 0.009(2) -0.002(2) -0.004(2)
C4 0.013(2) 0.025(2) 0.027(2) 0.006(2) 0.0039(19) 0.0032(18)
C5 0.026(3) 0.030(3) 0.029(3) 0.001(2) 0.009(2) 0.011(2)
C6 0.037(3) 0.024(3) 0.031(3) -0.006(2) -0.001(3) -0.005(2)
C7 0.021(3) 0.049(3) 0.035(3) -0.002(3) -0.012(2) -0.009(3)
C8 0.010(2) 0.025(2) 0.023(2) -0.002(2) -0.0011(18) 0.0014(19)
C9 0.011(2) 0.025(2) 0.032(3) -0.0008(19) 0.001(2) 0.000(2)
C10 0.020(3) 0.026(2) 0.023(2) 0.0001(18) 0.004(2) -0.005(2)
C11 0.018(2) 0.027(2) 0.020(2) -0.003(2) 0.003(2) -0.001(2)
C12 0.023(3) 0.032(3) 0.024(2) -0.002(2) 0.000(2) 0.002(2)
C13 0.028(3) 0.049(3) 0.030(3) -0.014(3) 0.009(2) -0.009(3)

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C10 C8 C9 107.0(4) . . ?
C4 C8 C9 114.0(4) . . ?
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