Assessment of intercomponent interaction in phenylene bridged dinuclear ruthenium(II) and osmium(II) polypyridyl complexes

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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
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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C47 C 0.5039(4) 0.2544(2) 0.7438(3) 0.0514(17) Uani 1 d . . .
H47 H 0.5244 0.2382 0.7815 0.051(6) Uiso 1 calc R . .
C48 C 0.4833(4) 0.2220(2) 0.6920(3) 0.0448(15) Uani 1 d . . .
H48 H 0.4894 0.1840 0.6948 0.051(6) Uiso 1 calc R . .
C49 C 0.4537(3) 0.2463(2) 0.6367(3) 0.0373(13) Uani 1 d . . .
H49 H 0.4403 0.2253 0.6011 0.051(6) Uiso 1 calc R . .
C50 C 0.4446(3) 0.3027(2) 0.6351(3) 0.0361(13) Uani 1 d . . .
H50 H 0.4238 0.3192 0.5976 0.051(6) Uiso 1 calc R . .
C51 C -0.0644(4) 0.1867(2) 0.7204(3) 0.0402(14) Uani 1 d . . .
H51 H -0.0045 0.1761 0.7239 0.058(7) Uiso 1 calc R . .
C52 C -0.1082(4) 0.1833(2) 0.7715(3) 0.0488(16) Uani 1 d . . .
H52 H -0.0784 0.1712 0.8089 0.058(7) Uiso 1 calc R . .
C53 C -0.1973(5) 0.1981(3) 0.7667(3) 0.0580(18) Uani 1 d . . .
H53 H -0.2287 0.1961 0.8009 0.058(7) Uiso 1 calc R . .
C54 C -0.2389(4) 0.2158(2) 0.7108(3) 0.0503(16) Uani 1 d . . .
H54 H -0.2993 0.2253 0.7066 0.058(7) Uiso 1 calc R . .
C55 C -0.1911(4) 0.2194(2) 0.6605(3) 0.0367(13) Uani 1 d . . .
C56 C -0.2288(4) 0.2386(2) 0.5990(3) 0.0376(14) Uani 1 d . . .
C57 C -0.3189(4) 0.2487(3) 0.5814(3) 0.0541(17) Uani 1 d . . .
H57 H -0.3599 0.2433 0.6095 0.058(7) Uiso 1 calc R . .
C58 C -0.3482(4) 0.2665(3) 0.5230(4) 0.062(2) Uani 1 d . . .
H58 H -0.4089 0.2726 0.5109 0.058(7) Uiso 1 calc R . .
C59 C -0.2861(4) 0.2752(3) 0.4822(3) 0.0618(19) Uani 1 d . . .
H59 H -0.3044 0.2883 0.4427 0.058(7) Uiso 1 calc R . .
C60 C -0.1956(4) 0.2641(2) 0.5007(3) 0.0477(16) Uani 1 d . . .
H60 H -0.1538 0.2697 0.4732 0.058(7) Uiso 1 calc R . .
C61 C 0.0353(4) 0.2080(3) 0.4652(3) 0.0443(15) Uani 1 d . . .
H61 H 0.0214 0.1709 0.4674 0.046(6) Uiso 1 calc R . .
C62 C 0.0744(4) 0.2267(3) 0.4146(3) 0.0522(17) Uani 1 d . . .
H62 H 0.0867 0.2026 0.3836 0.046(6) Uiso 1 calc R . .
C63 C 0.0948(4) 0.2817(3) 0.4115(3) 0.0562(17) Uani 1 d . . .
H63 H 0.1205 0.2954 0.3779 0.046(6) Uiso 1 calc R . .
C64 C 0.0766(4) 0.3168(3) 0.4586(3) 0.0493(16) Uani 1 d . . .
H64 H 0.0896 0.3540 0.4566 0.046(6) Uiso 1 calc R . .
C65 C 0.0389(3) 0.2958(2) 0.5089(3) 0.0350(13) Uani 1 d . . .
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C66 C 0.0205(3) 0.3281(2) 0.5623(2) 0.0328(13) Uani 1 d . . .
C67 C 0.0345(4) 0.3843(2) 0.5676(3) 0.0456(15) Uani 1 d . . .
H67 H 0.0541 0.4038 0.5351 0.046(6) Uiso 1 calc R . .
C68 C 0.0193(4) 0.4112(2) 0.6211(3) 0.0477(16) Uani 1 d . . .
H68 H 0.0279 0.4489 0.6250 0.046(6) Uiso 1 calc R . .
C69 C -0.0085(4) 0.3814(2) 0.6681(3) 0.0407(14) Uani 1 d . . .
H69 H -0.0183 0.3984 0.7049 0.046(6) Uiso 1 calc R . .
C70 C -0.0220(3) 0.3251(2) 0.6605(3) 0.0333(13) Uani 1 d . . .
H70 H -0.0421 0.3051 0.6925 0.046(6) Uiso 1 calc R . .
O100 O 0.1219(3) 0.37021(18) 0.2898(2) 0.0594(12) Uani 1 d . . .
C100 C 0.1210(4) 0.4169(3) 0.3060(3) 0.0499(16) Uani 1 d . . .
C101 C 0.1842(7) 0.4386(4) 0.3541(5) 0.171(6) Uani 1 d . . .
H10A H 0.2254 0.4102 0.3695 0.178(19) Uiso 1 calc R . .
H10B H 0.1530 0.4520 0.3870 0.178(19) Uiso 1 calc R . .
H10C H 0.2167 0.4682 0.3381 0.178(19) Uiso 1 calc R . .
C102 C 0.0528(5) 0.4568(3) 0.2775(4) 0.079(2) Uani 1 d . . .
H10D H 0.0140 0.4388 0.2454 0.178(19) Uiso 1 calc R . .
H10E H 0.0825 0.4870 0.2602 0.178(19) Uiso 1 calc R . .
H10F H 0.0180 0.4702 0.3084 0.178(19) Uiso 1 calc R . .
O200 O 0.1728(4) 0.1011(2) 0.4684(3) 0.0622(19) Uani 0.70 d P . .
C200 C 0.2496(5) 0.1091(3) 0.4762(4) 0.0359(19) Uani 0.70 d P . .
C201 C 0.2877(5) 0.1461(3) 0.5239(3) 0.039(2) Uani 0.70 d P . .
H20A H 0.2410 0.1599 0.5461 0.023(7) Uiso 0.70 calc PR . .
H20B H 0.3162 0.1762 0.5055 0.023(7) Uiso 0.70 calc PR . .
H20C H 0.3311 0.1268 0.5518 0.023(7) Uiso 0.70 calc PR . .
C202 C 0.3119(6) 0.0837(4) 0.4390(4) 0.066(3) Uani 0.70 d P . .
H20D H 0.2796 0.0600 0.4089 0.023(7) Uiso 0.70 calc PR . .
H20E H 0.3551 0.0626 0.4651 0.023(7) Uiso 0.70 calc PR . .
H20F H 0.3421 0.1117 0.4184 0.023(7) Uiso 0.70 calc PR . .

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_atom_site_aniso_U_13
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Ru2 0.0249(2) 0.0288(2) 0.0327(3) 0.00090(19) 0.00489(18) -0.00047(19)
P1 0.0678(13) 0.0624(12) 0.0544(12) -0.0035(10) 0.0027(10) -0.0063(10)
F11 0.115(3) 0.060(3) 0.066(3) -0.012(2) 0.012(2) -0.003(2)
F12 0.140(4) 0.115(4) 0.094(4) -0.038(3) 0.054(3) -0.062(3)
F13 0.100(3) 0.132(4) 0.059(3) 0.009(3) 0.003(2) 0.036(3)
F14 0.095(3) 0.095(3) 0.083(3) -0.038(3) 0.008(3) 0.008(3)
F15 0.074(3) 0.105(4) 0.173(5) -0.016(3) 0.046(3) -0.024(3)
F16 0.194(6) 0.067(3) 0.095(4) -0.008(3) -0.060(4) 0.025(3)
P2 0.0504(11) 0.0666(12) 0.0445(11) 0.0105(9) 0.0055(8) 0.0082(9)
F21 0.053(3) 0.172(5) 0.111(4) 0.048(3) 0.027(3) 0.026(3)
F24 0.054(2) 0.088(3) 0.093(3) 0.010(2) 0.016(2) -0.002(2)
F22 0.062(4) 0.073(5) 0.155(7) 0.059(5) 0.024(4) 0.015(3)
F23 0.092(5) 0.212(10) 0.052(5) -0.047(5) -0.008(4) 0.019(6)
F25 0.089(6) 0.082(6) 0.255(12) 0.090(7) -0.036(7) -0.010(5)
F26 0.149(8) 0.204(11) 0.099(7) -0.112(7) -0.039(5) 0.085(8)
P3 0.0443(9) 0.0393(9) 0.0364(9) -0.0009(7) 0.0041(7) 0.0054(7)
F32 0.128(4) 0.050(2) 0.100(3) 0.013(2) -0.043(3) 0.012(3)
F35 0.109(4) 0.051(2) 0.111(4) 0.002(2) -0.028(3) 0.028(2)
F31 0.094(4) 0.048(3) 0.066(3) -0.004(3) -0.027(3) -0.024(3)
F33 0.080(4) 0.168(7) 0.094(5) -0.005(5) 0.057(4) 0.006(5)
F34 0.114(5) 0.058(3) 0.070(4) -0.012(3) -0.045(4) -0.003(3)
F36 0.121(6) 0.156(7) 0.110(5) -0.031(5) 0.086(5) -0.045(5)
```

P4 0.0483(10) 0.0484(11) 0.0727(14) 0.0098(10) −0.0025(9) −0.0024(9)
F41 0.065(3) 0.062(3) 0.113(4) 0.035(2) 0.000(2) −0.001(2)
F44 0.090(3) 0.069(3) 0.118(4) 0.026(3) −0.013(3) 0.018(2)
F42 0.078(5) 0.089(6) 0.213(10) 0.083(6) −0.055(6) −0.054(4)
F43 0.137(6) 0.096(5) 0.026(3) −0.008(3) 0.013(3) 0.042(4)
F45 0.054(3) 0.067(4) 0.056(4) −0.015(3) −0.008(3) −0.018(3)
F46 0.084(5) 0.113(6) 0.118(6) 0.016(5) 0.055(5) 0.025(5)
N1 0.030(2) 0.025(2) 0.026(2) 0.0001(18) −0.0018(19) 0.0011(18)
N2 0.033(3) 0.040(3) 0.030(3) −0.001(2) 0.007(2) 0.001(2)
N3 0.039(3) 0.026(2) 0.029(3) −0.0019(19) 0.006(2) −0.003(2)
N4 0.026(2) 0.023(2) 0.034(3) −0.0003(19) 0.0072(19) −0.0058(18)
N5 0.027(2) 0.031(2) 0.033(3) 0.004(2) 0.005(2) 0.0052(19)
N6 0.029(2) 0.043(3) 0.040(3) −0.003(2) 0.007(2) −0.007(2)
N7 0.040(3) 0.025(2) 0.030(3) −0.0039(19) 0.003(2) −0.001(2)
N8 0.035(3) 0.030(2) 0.030(3) 0.002(2) 0.007(2) −0.004(2)
N9 0.028(2) 0.032(2) 0.029(3) 0.0008(19) 0.0071(19) −0.0011(19)
N10 0.029(2) 0.028(2) 0.027(2) −0.003(2) 0.0080(19) 0.0024(19)
N11 0.030(2) 0.033(3) 0.035(3) 0.000(2) 0.007(2) −0.001(2)
N12 0.031(3) 0.034(3) 0.040(3) 0.002(2) 0.002(2) 0.001(2)
N13 0.031(2) 0.038(3) 0.030(3) 0.001(2) 0.005(2) 0.001(2)
N14 0.025(2) 0.026(2) 0.031(3) 0.001(2) 0.0030(19) 0.0042(18)
C1 0.033(3) 0.030(3) 0.021(3) 0.001(2) 0.004(2) 0.004(2)
C2 0.034(3) 0.053(4) 0.032(3) −0.005(3) 0.009(3) −0.004(3)
C3 0.045(4) 0.073(5) 0.049(4) −0.004(4) 0.019(3) 0.000(4)
C4 0.045(4) 0.065(5) 0.053(4) −0.018(3) 0.014(3) 0.019(3)
C5 0.050(4) 0.043(4) 0.046(4) −0.013(3) 0.003(3) 0.004(3)
C6 0.035(3) 0.033(3) 0.033(3) −0.002(2) 0.006(3) 0.004(2)
C7 0.036(3) 0.024(3) 0.025(3) −0.004(2) 0.001(2) 0.001(2)
C8 0.047(3) 0.022(3) 0.025(3) −0.004(2) 0.000(2) −0.005(2)
C9 0.057(4) 0.031(3) 0.040(4) −0.007(3) −0.002(3) 0.001(3)
C10 0.079(5) 0.022(3) 0.055(4) 0.001(3) −0.007(4) −0.006(3)
C11 0.067(5) 0.036(4) 0.047(4) 0.003(3) 0.002(3) −0.019(3)
C12 0.055(4) 0.034(3) 0.036(3) −0.004(3) 0.011(3) −0.008(3)
C13 0.027(3) 0.027(3) 0.036(3) 0.004(2) 0.007(2) −0.003(2)
C14 0.044(3) 0.043(3) 0.025(3) 0.003(3) 0.004(3) −0.012(3)
C15 0.042(3) 0.040(3) 0.028(3) 0.014(3) 0.000(3) −0.007(3)
C16 0.020(3) 0.036(3) 0.032(3) −0.001(2) 0.003(2) −0.002(2)
C17 0.032(3) 0.037(3) 0.025(3) 0.000(2) 0.001(2) −0.002(3)
C18 0.035(3) 0.026(3) 0.035(3) 0.007(2) 0.007(2) −0.006(2)
C19 0.032(3) 0.027(3) 0.035(3) 0.006(2) 0.008(2) 0.000(2)
C20 0.037(4) 0.053(4) 0.056(4) 0.005(3) −0.005(3) 0.005(3)
C21 0.052(4) 0.055(4) 0.069(5) 0.011(4) −0.012(4) 0.018(4)
C22 0.069(5) 0.039(4) 0.075(5) 0.001(3) 0.006(4) 0.023(4)
C23 0.045(4) 0.030(3) 0.056(4) 0.005(3) 0.000(3) 0.006(3)
C24 0.034(3) 0.029(3) 0.038(3) 0.005(2) 0.012(3) 0.001(2)
C25 0.033(3) 0.025(3) 0.035(3) 0.002(2) 0.012(2) 0.001(2)
C26 0.033(3) 0.027(3) 0.037(3) −0.002(2) 0.018(2) −0.005(2)
C27 0.046(4) 0.033(3) 0.044(4) −0.008(3) 0.020(3) −0.003(3)
C28 0.045(4) 0.047(4) 0.056(4) −0.021(3) 0.022(3) −0.018(3)
C29 0.037(4) 0.060(4) 0.061(4) −0.025(3) 0.012(3) −0.016(3)
C30 0.032(3) 0.053(4) 0.046(4) −0.009(3) 0.010(3) −0.008(3)
C31 0.034(3) 0.037(3) 0.030(3) 0.002(2) 0.000(2) 0.000(2)
C32 0.044(4) 0.052(4) 0.031(3) 0.004(3) 0.002(3) 0.002(3)
C33 0.058(4) 0.071(5) 0.027(4) 0.007(3) −0.006(3) −0.010(4)
C34 0.058(4) 0.062(4) 0.027(3) 0.000(3) 0.008(3) −0.010(3)
C35 0.043(3) 0.036(3) 0.032(3) 0.001(3) 0.011(3) 0.001(3)
C36 0.037(3) 0.034(3) 0.030(3) 0.004(2) 0.009(2) −0.002(3)
C37 0.050(4) 0.057(4) 0.042(4) −0.001(3) 0.024(3) 0.000(3)
C38 0.042(4) 0.068(5) 0.059(5) 0.005(4) 0.024(3) 0.009(3)
C39 0.028(3) 0.070(5) 0.060(5) 0.006(3) 0.008(3) 0.003(3)
C40 0.039(3) 0.049(4) 0.036(4) 0.002(3) 0.000(3) −0.005(3)

```
C41 0.045(3) 0.036(3) 0.030(3) -0.005(3) 0.003(3) 0.000(3)
C42 0.059(4) 0.046(4) 0.026(3) -0.003(3) 0.002(3) -0.002(3)
C43 0.085(5) 0.061(5) 0.024(4) 0.002(3) -0.004(3) 0.003(4)
C44 0.072(5) 0.044(4) 0.035(4) 0.004(3) 0.001(3) 0.003(3)
C45 0.044(3) 0.028(3) 0.034(3) 0.004(2) 0.002(3) 0.002(3)
C46 0.039(3) 0.029(3) 0.029(3) 0.007(2) 0.006(2) 0.007(2)
C47 0.071(5) 0.030(3) 0.052(4) 0.008(3) 0.003(3) 0.015(3)
C48 0.051(4) 0.024(3) 0.060(4) -0.007(3) 0.008(3) -0.001(3)
C49 0.032(3) 0.036(3) 0.045(4) -0.008(3) 0.009(3) 0.002(3)
C50 0.037(3) 0.035(3) 0.037(3) -0.003(3) 0.007(3) 0.000(3)
C51 0.036(3) 0.041(3) 0.043(4) 0.009(3) 0.006(3) -0.001(3)
C52 0.055(4) 0.054(4) 0.039(4) 0.009(3) 0.012(3) -0.001(3)
C53 0.071(5) 0.060(4) 0.049(4) 0.008(3) 0.031(4) -0.008(4)
C54 0.033(3) 0.052(4) 0.069(5) -0.002(3) 0.021(3) -0.003(3)
C55 0.034(3) 0.030(3) 0.048(4) 0.003(3) 0.013(3) -0.008(3)
C56 0.030(3) 0.030(3) 0.053(4) 0.000(3) 0.006(3) 0.000(2)
C57 0.031(3) 0.061(4) 0.070(5) 0.008(4) 0.006(3) 0.006(3)
C58 0.025(3) 0.069(5) 0.086(6) 0.002(4) -0.011(4) 0.001(3)
C59 0.047(4) 0.074(5) 0.058(5) 0.016(4) -0.019(4) 0.008(4)
C60 0.041(4) 0.054(4) 0.045(4) 0.004(3) -0.005(3) 0.001(3)
C61 0.047(4) 0.049(4) 0.039(4) -0.002(3) 0.010(3) -0.001(3)
C62 0.061(4) 0.059(4) 0.040(4) -0.006(3) 0.020(3) 0.001(3)
C63 0.064(4) 0.065(5) 0.045(4) 0.008(4) 0.027(3) 0.000(4)
C64 0.060(4) 0.046(4) 0.043(4) 0.008(3) 0.010(3) 0.004(3)
C65 0.033(3) 0.037(3) 0.035(3) 0.010(3) 0.003(2) 0.005(2)
C66 0.033(3) 0.033(3) 0.032(3) 0.002(2) 0.004(2) 0.001(2)
C67 0.056(4) 0.033(3) 0.049(4) 0.008(3) 0.011(3) -0.002(3)
C68 0.058(4) 0.025(3) 0.061(4) -0.003(3) 0.010(3) 0.002(3)
C69 0.042(3) 0.037(3) 0.043(4) -0.004(3) 0.005(3) 0.006(3)
C70 0.030(3) 0.032(3) 0.037(3) -0.001(3) 0.002(2) 0.003(2)
O100 0.066(3) 0.046(3) 0.065(3) -0.008(2) 0.005(2) -0.003(2)
C100 0.055(4) 0.048(4) 0.046(4) -0.002(3) 0.001(3) 0.001(3)
C101 0.192(12) 0.076(7) 0.205(12) -0.037(7) -0.133(10) 0.007(7)
C102 0.082(6) 0.072(5) 0.084(6) 0.010(4) 0.013(5) 0.031(4)
O200 0.031(3) 0.035(3) 0.116(6) -0.022(3) -0.007(4) -0.003(3)
C200 0.036(5) 0.019(4) 0.051(5) -0.006(4) 0.000(4) 0.004(3)
C201 0.040(5) 0.048(5) 0.031(5) 0.000(4) 0.011(4) -0.015(4)
C202 0.049(6) 0.079(7) 0.060(7) -0.023(6) -0.025(5) 0.005(5)

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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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Ru1 N10 2.054(4) . ?
Ru1 N8 2.059(4) . ?
Ru1 N9 2.068(4) . ?
Ru1 N3 2.072(4) . ?
Ru1 N1 2.080(4) . ?
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Ru2 N12 2.049(4) . ?
Ru2 N11 2.050(4) . ?
Ru2 N13 2.054(4) . ?
Ru2 N14 2.067(4) . ?
Ru2 N6 2.081(4) . ?
Ru2 N4 2.086(4) . ?
P1 F16 1.562(4) . ?
P1 F15 1.576(5) . ?
P1 F14 1.577(4) . ?
P1 F13 1.585(4) . ?
P1 F12 1.585(5) . ?
P1 F11 1.605(4) . ?
P2 F23X 1.492(12) . ?
P2 F25X 1.524(12) . ?
P2 F22X 1.531(12) . ?
P2 F25 1.539(6) . ?
P2 F26 1.553(6) . ?
P2 F21 1.581(4) . ?
P2 F24 1.587(4) . ?
P2 F22 1.595(5) . ?
P2 F26X 1.603(12) . ?
P2 F23 1.604(6) . ?
F22 F23X 1.07(2) . ?
F22 F22X 1.565(16) . ?
F23 F23X 1.209(19) . ?
F23 F25X 1.228(17) . ?
F25 F25X 1.080(17) . ?
F25 F26X 1.151(18) . ?
F26 F22X 0.830(17) . ?
F26 F26X 1.429(18) . ?
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N7 C35 C36 114.8(5) . . ?
C34 C35 C36 124.3(5) . . ?
N8 C36 C37 121.0(5) . . ?
N8 C36 C35 114.2(5) . . ?
C37 C36 C35 124.7(5) . . ?
C38 C37 C36 119.4(6) . . ?
C37 C38 C39 120.3(6) . . ?
C40 C39 C38 119.3(6) . . ?
C39 C40 N8 122.5(5) . . ?
N9 C41 C42 123.8(5) . . ?
C43 C42 C41 118.8(5) . . ?
C42 C43 C44 119.1(6) . . ?
C45 C44 C43 119.6(6) . . ?
N9 C45 C44 121.6(5) . . ?
N9 C45 C46 114.2(4) . . ?
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N10 C46 C45 115.1(4) . . ?
C47 C46 C45 124.4(5) . . ?
C46 C47 C48 120.4(6) . . ?
C49 C48 C47 119.4(5) . . ?
C48 C49 C50 118.2(5) . . ?
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N11 C51 C52 123.4(5) . . ?
C51 C52 C53 118.9(6) . . ?
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C57 C56 C55 124.5(6) . . ?
C58 C57 C56 120.6(6) . . ?
C57 C58 C59 118.9(6) . . ?
C58 C59 C60 119.6(6) . . ?
N12 C60 C59 120.8(6) . . ?
N13 C61 C62 123.0(6) . . ?
C63 C62 C61 118.4(6) . . ?
C62 C63 C64 119.8(6) . . ?
C63 C64 C65 119.6(6) . . ?
N13 C65 C64 120.6(5) . . ?
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C64 C65 C66 124.5(5) . . ?
N14 C66 C67 121.0(5) . . ?
N14 C66 C65 115.1(5) . . ?
C67 C66 C65 123.8(5) . . ?
C68 C67 C66 119.9(5) . . ?
C69 C68 C67 118.7(5) . . ?
C68 C69 C70 119.2(5) . . ?
N14 C70 C69 122.6(5) . . ?
O100 C100 C101 122.7(7) . . ?
O100 C100 C102 122.0(6) . . ?
C101 C100 C102 115.3(7) . . ?
O200 C200 C201 120.7(8) . . ?
O200 C200 C202 122.9(8) . . ?
C201 C200 C202 116.4(7) . . ?

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_refine_diff_density_min         -1.014
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