Conformational studies of ligand-template assemblies and the consequences for encapsulation of rhodium complexes and hydroformylation catalysis

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#
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Crystal & Structural Chemistry
Padualaan 8, 3584CH Utrecht, The Netherlands
#
Note: The dataset has only limited resolution, related to the
high disordered solvent volume (4203 out of 19962 cubic Angstrom)
The disordered solvent contribution to the structure factors was taken
into account with the SQUEEZE procedure (see data at the end of this CIF)
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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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N2 N 0.29275(19) 0.1530(2) 0.09973(7) 0.0445(9) Uani 1 1 d . . .
N3 N 0.37873(19) 0.24509(18) 0.06421(6) 0.0374(8) Uani 1 1 d . . .
C1 C 0.0868(2) 0.0667(2) 0.04862(7) 0.0382(10) Uani 1 1 d . . .
C2 C 0.0921(2) 0.1126(2) 0.02898(8) 0.0463(11) Uani 1 1 d . . .
H2 H 0.0490 0.1117 0.0226 0.056 Uiso 1 1 calc R . .
C3 C 0.1605(2) 0.1598(2) 0.01861(8) 0.0451(11) Uani 1 1 d . . .
H3 H 0.1650 0.1924 0.0053 0.054 Uiso 1 1 calc R . .
C4 C 0.2224(2) 0.1595(2) 0.02769(8) 0.0407(11) Uani 1 1 d . . .
H4 H 0.2690 0.1910 0.0201 0.049 Uiso 1 1 calc R . .
C5 C 0.1520(2) 0.0714(2) 0.05696(7) 0.0411(11) Uani 1 1 d . . .

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C6 C 0.3164(2) 0.2287(2) 0.10358(8) 0.0433(11) Uani 1 1 d . . .
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C8 C 0.3862(2) 0.3530(2) 0.08715(8) 0.0444(11) Uani 1 1 d . . .
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C9 C 0.3680(3) 0.3802(3) 0.10807(9) 0.0497(12) Uani 1 1 d . . .
H9 H 0.3859 0.4318 0.1097 0.060 Uiso 1 1 calc R . .
C10 C 0.3235(3) 0.3319(3) 0.12672(9) 0.0520(12) Uani 1 1 d . . .
H10 H 0.3109 0.3503 0.1412 0.062 Uiso 1 1 calc R . .
C11 C 0.2976(2) 0.2574(3) 0.12430(9) 0.0507(12) Uani 1 1 d . . .
H11 H 0.2661 0.2246 0.1370 0.061 Uiso 1 1 calc R . .
C12 C 0.2555(2) 0.1021(3) 0.11641(9) 0.0515(12) Uani 1 1 d . . .
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C13 C 0.2283(3) 0.0240(3) 0.11338(9) 0.0527(13) Uani 1 1 d . . .
C14 C 0.1809(3) -0.0213(3) 0.13291(10) 0.0733(16) Uani 1 1 d . . .
H14 H 0.1704 0.0006 0.1469 0.088 Uiso 1 1 calc R . .
C15 C 0.1503(3) -0.0964(3) 0.13174(12) 0.0807(18) Uani 1 1 d . . .
H15 H 0.1183 -0.1269 0.1448 0.097 Uiso 1 1 calc R . .
C16 C 0.1662(3) -0.1275(3) 0.11127(11) 0.0775(17) Uani 1 1 d . . .
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C17 C 0.2126(3) -0.0880(3) 0.09190(10) 0.0606(14) Uani 1 1 d . . .
C18 C 0.2456(3) -0.0078(3) 0.09268(9) 0.0538(13) Uani 1 1 d . . .
C19 C 0.4284(2) 0.2845(2) 0.04761(8) 0.0405(11) Uani 1 1 d . . .
H19 H 0.4524 0.3366 0.0498 0.049 Uiso 1 1 calc R . .
C20 C 0.4517(2) 0.2586(2) 0.02620(8) 0.0382(10) Uani 1 1 d . . .
C21 C 0.4234(2) 0.1817(2) 0.02039(8) 0.0395(11) Uani 1 1 d . . .
C22 C 0.4562(2) 0.1638(2) -0.00045(8) 0.0439(11) Uani 1 1 d . . .
C23 C 0.5114(3) 0.2207(3) -0.01391(9) 0.0543(13) Uani 1 1 d . . .
H23 H 0.5327 0.2086 -0.0276 0.065 Uiso 1 1 calc R . .
C24 C 0.5382(3) 0.2956(3) -0.00864(9) 0.0578(13) Uani 1 1 d . . .
H24 H 0.5761 0.3330 -0.0187 0.069 Uiso 1 1 calc R . .
C25 C 0.5090(2) 0.3140(2) 0.01127(9) 0.0502(12) Uani 1 1 d . . .
H25 H 0.5273 0.3647 0.0152 0.060 Uiso 1 1 calc R . .
C26 C 0.2290(4) -0.1248(3) 0.06976(10) 0.0730(17) Uani 1 1 d . . .
C27 C 0.3109(4) -0.0996(3) 0.06839(11) 0.0825(18) Uani 1 1 d . . .
H27A H 0.3394 -0.0457 0.0665 0.124 Uiso 1 1 calc R . .
H27B H 0.3202 -0.1229 0.0538 0.124 Uiso 1 1 calc R . .
H27C H 0.3261 -0.1140 0.0839 0.124 Uiso 1 1 calc R . .
C28 C 0.2027(4) -0.1062(3) 0.04467(10) 0.090(2) Uani 1 1 d . . .
H28A H 0.2331 -0.0532 0.0411 0.134 Uiso 1 1 calc R . .
H28B H 0.1508 -0.1193 0.0463 0.134 Uiso 1 1 calc R . .
H28C H 0.2077 -0.1345 0.0308 0.134 Uiso 1 1 calc R . .
C29 C 0.1853(4) -0.2104(3) 0.07271(11) 0.107(2) Uani 1 1 d . . .
H29A H 0.1903 -0.2334 0.0572 0.160 Uiso 1 1 calc R . .
H29B H 0.1330 -0.2271 0.0757 0.160 Uiso 1 1 calc R . .
H29C H 0.2053 -0.2247 0.0870 0.160 Uiso 1 1 calc R . .
C30 C 0.4296(2) 0.0825(2) -0.00686(9) 0.0486(12) Uani 1 1 d . . .
C31 C 0.4725(3) 0.0754(3) -0.02935(9) 0.0588(13) Uani 1 1 d . . .
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H31C H 0.5255 0.1009 -0.0254 0.088 Uiso 1 1 calc R . .
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H32B H 0.4227 -0.0090 0.0118 0.082 Uiso 1 1 calc R . .

H32C H 0.4132 0.0458 0.0305 0.082 Uiso 1 1 calc R . .
C33 C 0.3472(3) 0.0415(2) -0.01374(9) 0.0595(14) Uani 1 1 d . . .
H33A H 0.3183 0.0419 0.0008 0.089 Uiso 1 1 calc R . .
H33B H 0.3317 -0.0097 -0.0183 0.089 Uiso 1 1 calc R . .
H33C H 0.3391 0.0662 -0.0281 0.089 Uiso 1 1 calc R . .
Zn2 Zn 0.49323(2) 0.40640(2) 0.157649(8) 0.03040(14) Uani 1 1 d . . .
P2 P 0.6667 0.3333 0.22641(3) 0.0304(4) Uani 1 3 d S . .
O3 O 0.42090(14) 0.31669(14) 0.17585(5) 0.0374(7) Uani 1 1 d . . .
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N5 N 0.50678(17) 0.34098(18) 0.13121(5) 0.0294(8) Uani 1 1 d . . .
N6 N 0.54737(17) 0.48347(18) 0.12849(5) 0.0321(8) Uani 1 1 d . . .
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C35 C 0.5973(2) 0.3872(2) 0.19264(7) 0.0300(9) Uani 1 1 d . . .
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C36 C 0.6130(2) 0.5040(2) 0.19478(7) 0.0364(10) Uani 1 1 d . . .
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C37 C 0.6651(2) 0.5239(2) 0.21383(8) 0.0412(11) Uani 1 1 d . . .
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C40 C 0.5686(2) 0.3487(2) 0.09016(7) 0.0389(10) Uani 1 1 d . . .
H40 H 0.5539 0.2976 0.0908 0.047 Uiso 1 1 calc R . .
C41 C 0.6085(2) 0.3908(3) 0.06971(7) 0.0422(11) Uani 1 1 d . . .
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C42 C 0.6312(2) 0.4651(3) 0.06866(8) 0.0427(11) Uani 1 1 d . . .
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C46 C 0.4265(2) 0.2223(2) 0.15214(7) 0.0317(9) Uani 1 1 d . . .
C47 C 0.3989(2) 0.2472(2) 0.17216(7) 0.0324(10) Uani 1 1 d . . .
C48 C 0.3430(2) 0.1926(2) 0.18854(7) 0.0362(10) Uani 1 1 d . . .
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H60C H 0.4107 0.3098 0.2198 0.085 Uiso 1 1 calc R . .
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H64B H 0.4243 0.6238 0.2273 0.112 Uiso 1 1 calc R . .
H64C H 0.3434 0.5545 0.2320 0.112 Uiso 1 1 calc R . .
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H65B H 0.4802 0.5440 0.2299 0.093 Uiso 1 1 calc R . .
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O1 0.071(2) 0.0351(18) 0.058(2) 0.0058(16) -0.0005(18) 0.0210(17)
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N3 0.038(2) 0.032(2) 0.044(2) -0.0035(18) -0.0128(18) 0.0186(18)
C1 0.039(3) 0.041(3) 0.036(2) -0.006(2) -0.007(2) 0.021(2)
C2 0.042(3) 0.052(3) 0.045(3) -0.004(2) -0.010(2) 0.023(2)
C3 0.042(3) 0.049(3) 0.038(3) 0.003(2) -0.004(2) 0.018(2)
C4 0.035(3) 0.040(3) 0.039(3) -0.007(2) -0.008(2) 0.013(2)
C5 0.049(3) 0.034(3) 0.035(2) -0.003(2) -0.009(2) 0.016(2)
C6 0.043(3) 0.048(3) 0.041(3) -0.011(2) -0.016(2) 0.025(2)
C7 0.039(3) 0.042(3) 0.042(3) -0.009(2) -0.016(2) 0.024(2)
C8 0.051(3) 0.043(3) 0.046(3) -0.007(2) -0.016(2) 0.028(2)
C9 0.054(3) 0.048(3) 0.055(3) -0.015(3) -0.021(3) 0.031(3)
C10 0.052(3) 0.065(4) 0.050(3) -0.017(3) -0.015(3) 0.037(3)
C11 0.046(3) 0.056(3) 0.049(3) 0.000(2) -0.009(2) 0.024(3)
C12 0.049(3) 0.055(3) 0.046(3) -0.002(3) -0.013(2) 0.023(3)
C13 0.047(3) 0.043(3) 0.053(3) 0.013(3) -0.010(2) 0.011(2)

C14 0.064(4) 0.066(4) 0.069(4) 0.006(3) -0.004(3) 0.017(3)
C15 0.078(4) 0.057(4) 0.077(4) 0.019(3) 0.008(3) 0.011(3)
C16 0.079(4) 0.043(3) 0.078(4) 0.002(3) -0.018(3) 0.007(3)
C17 0.066(3) 0.036(3) 0.059(3) 0.007(3) -0.021(3) 0.010(3)
C18 0.052(3) 0.051(3) 0.048(3) -0.001(3) -0.019(3) 0.018(3)
C19 0.039(3) 0.032(2) 0.052(3) -0.004(2) -0.016(2) 0.019(2)
C20 0.042(3) 0.034(3) 0.041(3) -0.003(2) -0.009(2) 0.021(2)
C21 0.033(3) 0.031(3) 0.053(3) -0.004(2) -0.016(2) 0.016(2)
C22 0.042(3) 0.044(3) 0.053(3) -0.010(2) -0.013(2) 0.027(2)
C23 0.049(3) 0.057(3) 0.058(3) -0.012(3) -0.002(3) 0.027(3)
C24 0.056(3) 0.042(3) 0.063(3) -0.006(3) 0.002(3) 0.016(3)
C25 0.054(3) 0.032(3) 0.059(3) -0.006(2) -0.005(3) 0.018(2)
C26 0.110(5) 0.034(3) 0.054(3) -0.001(2) -0.016(3) 0.020(3)
C27 0.115(5) 0.061(4) 0.074(4) -0.001(3) -0.007(4) 0.045(4)
C28 0.126(5) 0.056(4) 0.061(4) -0.008(3) -0.033(4) 0.026(4)
C29 0.166(7) 0.037(3) 0.087(4) 0.000(3) -0.007(4) 0.028(4)
C30 0.054(3) 0.044(3) 0.057(3) -0.011(2) -0.020(2) 0.030(2)
C31 0.069(3) 0.056(3) 0.065(3) -0.017(3) -0.016(3) 0.041(3)
C32 0.061(3) 0.040(3) 0.072(3) -0.013(2) -0.017(3) 0.032(3)
C33 0.060(3) 0.048(3) 0.074(3) -0.020(3) -0.029(3) 0.030(3)
Zn2 0.0345(3) 0.0331(3) 0.0271(3) -0.0024(2) 0.0000(2) 0.0195(2)
P2 0.0326(6) 0.0326(6) 0.0258(10) 0.000 0.000 0.0163(3)
O3 0.0417(17) 0.0347(17) 0.0359(16) -0.0033(13) 0.0065(13) 0.0191(14)
O4 0.0419(17) 0.0381(18) 0.0405(17) -0.0014(13) 0.0032(13) 0.0249(15)
N4 0.0332(19) 0.030(2) 0.0293(18) -0.0043(16) -0.0007(15) 0.0164(17)
N5 0.0295(19) 0.033(2) 0.0280(18) -0.0034(15) -0.0006(15) 0.0173(16)
N6 0.039(2) 0.034(2) 0.0286(18) -0.0002(15) -0.0027(15) 0.0215(17)
C34 0.031(2) 0.033(2) 0.021(2) 0.0001(17) 0.0038(18) 0.0168(19)
C35 0.033(2) 0.029(2) 0.028(2) -0.0038(18) 0.0017(19) 0.016(2)
C36 0.040(3) 0.034(3) 0.038(2) 0.004(2) 0.005(2) 0.021(2)
C37 0.048(3) 0.032(2) 0.038(3) -0.006(2) -0.010(2) 0.016(2)
C38 0.036(2) 0.036(3) 0.029(2) -0.0041(19) -0.0113(19) 0.015(2)
C39 0.026(2) 0.044(3) 0.024(2) -0.0036(19) -0.0044(18) 0.020(2)
C40 0.038(3) 0.045(3) 0.034(2) -0.007(2) 0.002(2) 0.021(2)
C41 0.037(3) 0.065(3) 0.030(2) -0.009(2) 0.002(2) 0.029(2)
C42 0.038(3) 0.062(3) 0.032(2) 0.011(2) 0.005(2) 0.027(2)
C43 0.043(3) 0.047(3) 0.037(3) 0.004(2) 0.005(2) 0.027(2)
C44 0.030(2) 0.042(3) 0.025(2) -0.0034(19) -0.0047(18) 0.021(2)
C45 0.035(2) 0.041(3) 0.034(2) -0.012(2) -0.008(2) 0.024(2)
C46 0.032(2) 0.037(3) 0.029(2) -0.0020(19) -0.0023(19) 0.019(2)
C47 0.030(2) 0.037(3) 0.032(2) -0.004(2) -0.0051(19) 0.018(2)
C48 0.034(2) 0.036(3) 0.036(2) 0.002(2) 0.000(2) 0.016(2)
C49 0.039(3) 0.044(3) 0.043(3) 0.007(2) 0.003(2) 0.013(2)
C50 0.057(3) 0.027(2) 0.046(3) -0.002(2) -0.005(2) 0.018(2)
C51 0.051(3) 0.041(3) 0.036(2) -0.005(2) -0.003(2) 0.028(2)
C52 0.050(3) 0.040(3) 0.032(2) 0.005(2) 0.001(2) 0.023(2)
C53 0.053(3) 0.038(3) 0.040(3) -0.004(2) 0.001(2) 0.027(2)
C54 0.084(4) 0.048(3) 0.055(3) 0.003(3) 0.017(3) 0.035(3)
C55 0.116(5) 0.041(3) 0.079(4) -0.002(3) 0.028(4) 0.042(3)
C56 0.089(4) 0.050(3) 0.069(4) -0.005(3) 0.020(3) 0.043(3)
C57 0.059(3) 0.039(3) 0.043(3) -0.006(2) -0.001(2) 0.032(2)
C58 0.043(3) 0.038(3) 0.038(2) -0.006(2) -0.004(2) 0.026(2)
C59 0.046(3) 0.050(3) 0.040(3) 0.004(2) 0.012(2) 0.023(2)
C60 0.067(3) 0.070(3) 0.038(3) -0.010(2) 0.004(2) 0.037(3)

C61 0.068(4) 0.066(3) 0.057(3) 0.013(3) 0.030(3) 0.028(3)
C62 0.049(3) 0.074(4) 0.063(3) 0.007(3) 0.017(2) 0.038(3)
C63 0.053(3) 0.048(3) 0.052(3) -0.012(2) 0.008(2) 0.028(3)
C64 0.084(4) 0.068(4) 0.076(4) -0.017(3) 0.021(3) 0.042(3)
C65 0.067(3) 0.076(4) 0.041(3) 0.008(3) 0.012(3) 0.035(3)
C66 0.045(3) 0.063(3) 0.088(4) -0.013(3) 0.010(3) 0.029(3)

_geom_special_details
;
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.
;

loop_
_geom_bond_atom_site_label_1
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Zn1 O1 1.947(3) . ?
Zn1 O2 1.960(3) . ?
Zn1 N3 2.074(3) . ?
Zn1 N2 2.092(4) . ?
Zn1 N1 2.131(3) . ?
P1 C1 1.847(4) 2 ?
P1 C1 1.847(4) . ?
P1 C1 1.847(4) 3 ?
O1 C18 1.291(5) . ?
O2 C21 1.291(5) . ?
N1 C5 1.335(5) . ?
N1 C4 1.339(5) . ?
N2 C12 1.298(5) . ?
N2 C6 1.415(5) . ?
N3 C19 1.293(5) . ?
N3 C7 1.413(5) . ?
C1 C2 1.380(6) . ?
C1 C5 1.386(5) . ?
C2 C3 1.380(6) . ?
C2 H2 0.9500 . ?
C3 C4 1.380(6) . ?
C3 H3 0.9500 . ?
C4 H4 0.9500 . ?
C5 H5 0.9500 . ?
C6 C11 1.397(6) . ?
C6 C7 1.404(6) . ?
C7 C8 1.398(6) . ?
C8 C9 1.382(6) . ?
C8 H8 0.9500 . ?
C9 C10 1.385(6) . ?
C9 H9 0.9500 . ?

C10 C11 1.373(6) . ?
C10 H10 0.9500 . ?
C11 H11 0.9500 . ?
C12 C13 1.442(6) . ?
C12 H12 0.9500 . ?
C13 C14 1.417(7) . ?
C13 C18 1.419(7) . ?
C14 C15 1.365(7) . ?
C14 H14 0.9500 . ?
C15 C16 1.388(8) . ?
C15 H15 0.9500 . ?
C16 C17 1.368(7) . ?
C16 H16 0.9500 . ?
C17 C18 1.456(6) . ?
C17 C26 1.531(7) . ?
C19 C20 1.440(6) . ?
C19 H19 0.9500 . ?
C20 C25 1.417(6) . ?
C20 C21 1.440(5) . ?
C21 C22 1.443(6) . ?
C22 C23 1.370(6) . ?
C22 C30 1.537(6) . ?
C23 C24 1.400(6) . ?
C23 H23 0.9500 . ?
C24 C25 1.365(6) . ?
C24 H24 0.9500 . ?
C25 H25 0.9500 . ?
C26 C27 1.519(8) . ?
C26 C29 1.555(7) . ?
C26 C28 1.558(7) . ?
C27 H27A 0.9800 . ?
C27 H27B 0.9800 . ?
C27 H27C 0.9800 . ?
C28 H28A 0.9800 . ?
C28 H28B 0.9800 . ?
C28 H28C 0.9800 . ?
C29 H29A 0.9800 . ?
C29 H29B 0.9800 . ?
C29 H29C 0.9800 . ?
C30 C33 1.533(6) . ?
C30 C31 1.541(6) . ?
C30 C32 1.545(6) . ?
C31 H31A 0.9800 . ?
C31 H31B 0.9800 . ?
C31 H31C 0.9800 . ?
C32 H32A 0.9800 . ?
C32 H32B 0.9800 . ?
C32 H32C 0.9800 . ?
C33 H33A 0.9800 . ?
C33 H33B 0.9800 . ?
C33 H33C 0.9800 . ?
Zn2 O4 1.959(3) . ?
Zn2 O3 1.971(3) . ?
Zn2 N5 2.071(3) . ?

Zn2 N6 2.105(3) . ?
Zn2 N4 2.114(3) . ?
P2 C34 1.826(4) . ?
P2 C34 1.827(4) 3_665 ?
P2 C34 1.827(4) 2_655 ?
O3 C47 1.298(4) . ?
O4 C58 1.300(5) . ?
N4 C36 1.335(5) . ?
N4 C35 1.344(5) . ?
N5 C45 1.297(5) . ?
N5 C39 1.423(5) . ?
N6 C52 1.286(5) . ?
N6 C44 1.417(5) . ?
C34 C35 1.384(5) . ?
C34 C38 1.393(5) . ?
C35 H35 0.9500 . ?
C36 C37 1.386(5) . ?
C36 H36 0.9500 . ?
C37 C38 1.369(5) . ?
C37 H37 0.9500 . ?
C38 H38 0.9500 . ?
C39 C40 1.392(5) . ?
C39 C44 1.410(5) . ?
C40 C41 1.381(6) . ?
C40 H40 0.9500 . ?
C41 C42 1.377(6) . ?
C41 H41 0.9500 . ?
C42 C43 1.368(6) . ?
C42 H42 0.9500 . ?
C43 C44 1.395(5) . ?
C43 H43 0.9500 . ?
C45 C46 1.441(5) . ?
C45 H45 0.9500 . ?
C46 C51 1.412(5) . ?
C46 C47 1.422(5) . ?
C47 C48 1.443(5) . ?
C48 C49 1.375(6) . ?
C48 C59 1.534(6) . ?
C49 C50 1.398(6) . ?
C49 H49 0.9500 . ?
C50 C51 1.361(6) . ?
C50 H50 0.9500 . ?
C51 H51 0.9500 . ?
C52 C53 1.432(6) . ?
C52 H52 0.9500 . ?
C53 C54 1.424(6) . ?
C53 C58 1.429(6) . ?
C54 C55 1.359(6) . ?
C54 H54 0.9500 . ?
C55 C56 1.401(7) . ?
C55 H55 0.9500 . ?
C56 C57 1.381(6) . ?
C56 H56 0.9500 . ?
C57 C58 1.435(5) . ?

C57 C63 1.541(6) . ?
C59 C61 1.533(6) . ?
C59 C62 1.539(6) . ?
C59 C60 1.540(6) . ?
C60 H60A 0.9800 . ?
C60 H60B 0.9800 . ?
C60 H60C 0.9800 . ?
C61 H61A 0.9800 . ?
C61 H61B 0.9800 . ?
C61 H61C 0.9800 . ?
C62 H62A 0.9800 . ?
C62 H62B 0.9800 . ?
C62 H62C 0.9800 . ?
C63 C66 1.527(6) . ?
C63 C64 1.528(6) . ?
C63 C65 1.531(6) . ?
C64 H64A 0.9800 . ?
C64 H64B 0.9800 . ?
C64 H64C 0.9800 . ?
C65 H65A 0.9800 . ?
C65 H65B 0.9800 . ?
C65 H65C 0.9800 . ?
C66 H66A 0.9800 . ?
C66 H66B 0.9800 . ?
C66 H66C 0.9800 . ?

loop_
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O1 Zn1 O2 95.89(13) . . ?
O1 Zn1 N3 155.18(13) . . ?
O2 Zn1 N3 89.92(13) . . ?
O1 Zn1 N2 89.41(14) . . ?
O2 Zn1 N2 163.05(13) . . ?
N3 Zn1 N2 78.87(14) . . ?
O1 Zn1 N1 103.42(13) . . ?
O2 Zn1 N1 99.85(12) . . ?
N3 Zn1 N1 99.29(13) . . ?
N2 Zn1 N1 94.53(13) . . ?
C1 P1 C1 100.69(16) 2 . ?
C1 P1 C1 100.69(16) 2 3 ?
C1 P1 C1 100.70(16) . 3 ?
C18 O1 Zn1 128.7(3) . . ?
C21 O2 Zn1 132.3(3) . . ?
C5 N1 C4 117.7(4) . . ?
C5 N1 Zn1 122.0(3) . . ?
C4 N1 Zn1 119.7(3) . . ?
C12 N2 C6 123.2(4) . . ?
C12 N2 Zn1 123.4(3) . . ?

C6 N2 Zn1 113.3(3) . . ?
C19 N3 C7 122.0(4) . . ?
C19 N3 Zn1 124.0(3) . . ?
C7 N3 Zn1 114.0(3) . . ?
C2 C1 C5 117.1(4) . . ?
C2 C1 P1 125.2(3) . . ?
C5 C1 P1 117.7(3) . . ?
C3 C2 C1 119.4(4) . . ?
C3 C2 H2 120.3 . . ?
C1 C2 H2 120.3 . . ?
C2 C3 C4 119.6(4) . . ?
C2 C3 H3 120.2 . . ?
C4 C3 H3 120.2 . . ?
N1 C4 C3 121.9(4) . . ?
N1 C4 H4 119.1 . . ?
C3 C4 H4 119.1 . . ?
N1 C5 C1 124.3(4) . . ?
N1 C5 H5 117.9 . . ?
C1 C5 H5 117.9 . . ?
C11 C6 C7 118.8(4) . . ?
C11 C6 N2 125.2(4) . . ?
C7 C6 N2 116.1(4) . . ?
C8 C7 C6 119.0(4) . . ?
C8 C7 N3 125.0(4) . . ?
C6 C7 N3 116.0(4) . . ?
C9 C8 C7 121.1(4) . . ?
C9 C8 H8 119.4 . . ?
C7 C8 H8 119.4 . . ?
C8 C9 C10 119.7(4) . . ?
C8 C9 H9 120.1 . . ?
C10 C9 H9 120.1 . . ?
C11 C10 C9 119.9(4) . . ?
C11 C10 H10 120.1 . . ?
C9 C10 H10 120.1 . . ?
C10 C11 C6 121.5(5) . . ?
C10 C11 H11 119.2 . . ?
C6 C11 H11 119.2 . . ?
N2 C12 C13 125.8(4) . . ?
N2 C12 H12 117.1 . . ?
C13 C12 H12 117.1 . . ?
C14 C13 C18 120.5(5) . . ?
C14 C13 C12 114.9(5) . . ?
C18 C13 C12 124.6(4) . . ?
C15 C14 C13 120.2(6) . . ?
C15 C14 H14 119.9 . . ?
C13 C14 H14 119.9 . . ?
C14 C15 C16 119.2(5) . . ?
C14 C15 H15 120.4 . . ?
C16 C15 H15 120.4 . . ?
C17 C16 C15 124.5(5) . . ?
C17 C16 H16 117.8 . . ?
C15 C16 H16 117.8 . . ?
C16 C17 C18 117.2(5) . . ?
C16 C17 C26 122.7(5) . . ?

C18 C17 C26 120.2(5) . . ?
O1 C18 C13 122.9(4) . . ?
O1 C18 C17 118.7(5) . . ?
C13 C18 C17 118.4(5) . . ?
N3 C19 C20 127.6(4) . . ?
N3 C19 H19 116.2 . . ?
C20 C19 H19 116.2 . . ?
C25 C20 C21 119.9(4) . . ?
C25 C20 C19 116.0(4) . . ?
C21 C20 C19 124.0(4) . . ?
O2 C21 C20 122.0(4) . . ?
O2 C21 C22 120.0(4) . . ?
C20 C21 C22 117.9(4) . . ?
C23 C22 C21 118.5(4) . . ?
C23 C22 C30 121.7(4) . . ?
C21 C22 C30 119.9(4) . . ?
C22 C23 C24 123.9(5) . . ?
C22 C23 H23 118.1 . . ?
C24 C23 H23 118.1 . . ?
C25 C24 C23 118.8(5) . . ?
C25 C24 H24 120.6 . . ?
C23 C24 H24 120.6 . . ?
C24 C25 C20 121.0(4) . . ?
C24 C25 H25 119.5 . . ?
C20 C25 H25 119.5 . . ?
C27 C26 C17 111.0(4) . . ?
C27 C26 C29 108.3(5) . . ?
C17 C26 C29 110.5(5) . . ?
C27 C26 C28 110.4(5) . . ?
C17 C26 C28 109.5(5) . . ?
C29 C26 C28 107.1(4) . . ?
C26 C27 H27A 109.5 . . ?
C26 C27 H27B 109.5 . . ?
H27A C27 H27B 109.5 . . ?
C26 C27 H27C 109.5 . . ?
H27A C27 H27C 109.5 . . ?
H27B C27 H27C 109.5 . . ?
C26 C28 H28A 109.5 . . ?
C26 C28 H28B 109.5 . . ?
H28A C28 H28B 109.5 . . ?
C26 C28 H28C 109.5 . . ?
H28A C28 H28C 109.5 . . ?
H28B C28 H28C 109.5 . . ?
C26 C29 H29A 109.5 . . ?
C26 C29 H29B 109.5 . . ?
H29A C29 H29B 109.5 . . ?
C26 C29 H29C 109.5 . . ?
H29A C29 H29C 109.5 . . ?
H29B C29 H29C 109.5 . . ?
C33 C30 C22 110.6(3) . . ?
C33 C30 C31 107.8(4) . . ?
C22 C30 C31 111.7(4) . . ?
C33 C30 C32 108.4(4) . . ?
C22 C30 C32 110.4(3) . . ?

C31 C30 C32 107.7(4) . . ?
C30 C31 H31A 109.5 . . ?
C30 C31 H31B 109.5 . . ?
H31A C31 H31B 109.5 . . ?
C30 C31 H31C 109.5 . . ?
H31A C31 H31C 109.5 . . ?
H31B C31 H31C 109.5 . . ?
C30 C32 H32A 109.5 . . ?
C30 C32 H32B 109.5 . . ?
H32A C32 H32B 109.5 . . ?
C30 C32 H32C 109.5 . . ?
H32A C32 H32C 109.5 . . ?
H32B C32 H32C 109.5 . . ?
C30 C33 H33A 109.5 . . ?
C30 C33 H33B 109.5 . . ?
H33A C33 H33B 109.5 . . ?
C30 C33 H33C 109.5 . . ?
H33A C33 H33C 109.5 . . ?
H33B C33 H33C 109.5 . . ?
O4 Zn2 O3 96.47(11) . . ?
O4 Zn2 N5 153.37(11) . . ?
O3 Zn2 N5 89.81(11) . . ?
O4 Zn2 N6 87.49(12) . . ?
O3 Zn2 N6 161.42(11) . . ?
N5 Zn2 N6 79.02(12) . . ?
O4 Zn2 N4 99.43(11) . . ?
O3 Zn2 N4 95.45(11) . . ?
N5 Zn2 N4 105.71(12) . . ?
N6 Zn2 N4 101.82(12) . . ?
C34 P2 C34 103.31(14) . 3_665 ?
C34 P2 C34 103.31(14) . 2_655 ?
C34 P2 C34 103.30(14) 3_665 2_655 ?
C47 O3 Zn2 131.5(2) . . ?
C58 O4 Zn2 130.1(2) . . ?
C36 N4 C35 117.8(3) . . ?
C36 N4 Zn2 121.1(3) . . ?
C35 N4 Zn2 120.8(2) . . ?
C45 N5 C39 121.4(3) . . ?
C45 N5 Zn2 124.3(3) . . ?
C39 N5 Zn2 114.2(2) . . ?
C52 N6 C44 121.8(3) . . ?
C52 N6 Zn2 124.1(3) . . ?
C44 N6 Zn2 114.0(2) . . ?
C35 C34 C38 117.1(3) . . ?
C35 C34 P2 125.4(3) . . ?
C38 C34 P2 117.3(3) . . ?
N4 C35 C34 123.6(3) . . ?
N4 C35 H35 118.2 . . ?
C34 C35 H35 118.2 . . ?
N4 C36 C37 122.7(4) . . ?
N4 C36 H36 118.6 . . ?
C37 C36 H36 118.6 . . ?
C38 C37 C36 118.5(4) . . ?
C38 C37 H37 120.7 . . ?

C36 C37 H37 120.7 . . ?
C37 C38 C34 120.2(4) . . ?
C37 C38 H38 119.9 . . ?
C34 C38 H38 119.9 . . ?
C40 C39 C44 118.8(4) . . ?
C40 C39 N5 124.4(4) . . ?
C44 C39 N5 116.7(3) . . ?
C41 C40 C39 120.5(4) . . ?
C41 C40 H40 119.8 . . ?
C39 C40 H40 119.8 . . ?
C42 C41 C40 120.4(4) . . ?
C42 C41 H41 119.8 . . ?
C40 C41 H41 119.8 . . ?
C43 C42 C41 120.2(4) . . ?
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C41 C42 H42 119.9 . . ?
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C44 C43 H43 119.6 . . ?
C43 C44 C39 119.3(4) . . ?
C43 C44 N6 125.3(4) . . ?
C39 C44 N6 115.3(3) . . ?
N5 C45 C46 127.1(4) . . ?
N5 C45 H45 116.4 . . ?
C46 C45 H45 116.4 . . ?
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C51 C46 C45 115.5(3) . . ?
C47 C46 C45 124.4(4) . . ?
O3 C47 C46 122.6(4) . . ?
O3 C47 C48 119.0(3) . . ?
C46 C47 C48 118.4(4) . . ?
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C56 C57 C58 117.8(4) . . ?
C56 C57 C63 122.5(4) . . ?
C58 C57 C63 119.6(4) . . ?
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O4 C58 C57 118.8(4) . . ?
C53 C58 C57 118.7(4) . . ?
C61 C59 C48 111.5(4) . . ?
C61 C59 C62 107.1(4) . . ?
C48 C59 C62 110.1(3) . . ?
C61 C59 C60 108.4(4) . . ?
C48 C59 C60 109.4(3) . . ?
C62 C59 C60 110.3(4) . . ?
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H60A C60 H60C 109.5 . . ?
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H61A C61 H61B 109.5 . . ?
C59 C61 H61C 109.5 . . ?
H61A C61 H61C 109.5 . . ?
H61B C61 H61C 109.5 . . ?
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H62A C62 H62B 109.5 . . ?
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H62A C62 H62C 109.5 . . ?
H62B C62 H62C 109.5 . . ?
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C66 C63 C65 110.4(4) . . ?
C64 C63 C65 108.1(4) . . ?
C66 C63 C57 110.4(4) . . ?
C64 C63 C57 111.4(4) . . ?
C65 C63 C57 109.7(4) . . ?
C63 C64 H64A 109.5 . . ?
C63 C64 H64B 109.5 . . ?
H64A C64 H64B 109.5 . . ?
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H64A C64 H64C 109.5 . . ?
H64B C64 H64C 109.5 . . ?
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C63 C65 H65B 109.5 . . ?
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N1 Zn1 O1 C18 -68.5(4) . . . . ?
O1 Zn1 O2 C21 -154.3(3) . . . . ?
N3 Zn1 O2 C21 1.5(3) . . . . ?
N2 Zn1 O2 C21 -46.7(6) . . . . ?
N1 Zn1 O2 C21 101.0(3) . . . . ?
O1 Zn1 N1 C5 39.8(3) . . . . ?
O2 Zn1 N1 C5 138.4(3) . . . . ?
N3 Zn1 N1 C5 -130.1(3) . . . . ?
N2 Zn1 N1 C5 -50.6(3) . . . . ?
O1 Zn1 N1 C4 -149.0(3) . . . . ?
O2 Zn1 N1 C4 -50.5(3) . . . . ?
N3 Zn1 N1 C4 41.1(3) . . . . ?
N2 Zn1 N1 C4 120.5(3) . . . . ?
O1 Zn1 N2 C12 -14.6(3) . . . . ?
O2 Zn1 N2 C12 -123.2(5) . . . . ?
N3 Zn1 N2 C12 -172.6(4) . . . . ?
N1 Zn1 N2 C12 88.8(3) . . . . ?
O1 Zn1 N2 C6 169.2(3) . . . . ?
O2 Zn1 N2 C6 60.7(6) . . . . ?
N3 Zn1 N2 C6 11.2(3) . . . . ?
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N2 Zn1 N3 C19 168.1(3) . . . . ?
N1 Zn1 N3 C19 -99.1(3) . . . . ?
O1 Zn1 N3 C7 -74.8(4) . . . . ?
O2 Zn1 N3 C7 -178.8(3) . . . . ?
N2 Zn1 N3 C7 -11.6(3) . . . . ?
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C1 P1 C1 C2 -4.0(4) 2 . . . ?
C1 P1 C1 C2 99.2(3) 3 . . . ?
C1 P1 C1 C5 176.0(3) 2 . . . ?
C1 P1 C1 C5 -80.9(4) 3 . . . ?
C5 C1 C2 C3 0.3(6) . . . . ?
P1 C1 C2 C3 -179.7(3) . . . . ?

C1 C2 C3 C4 1.3(6) . . . . ?
C5 N1 C4 C3 1.1(6) . . . . ?
Zn1 N1 C4 C3 -170.4(3) . . . . ?
C2 C3 C4 N1 -2.1(6) . . . . ?
C4 N1 C5 C1 0.6(6) . . . . ?
Zn1 N1 C5 C1 171.9(3) . . . . ?
C2 C1 C5 N1 -1.3(6) . . . . ?
P1 C1 C5 N1 178.7(3) . . . . ?
C12 N2 C6 C11 -6.1(6) . . . . ?
Zn1 N2 C6 C11 170.1(3) . . . . ?
C12 N2 C6 C7 174.5(4) . . . . ?
Zn1 N2 C6 C7 -9.3(4) . . . . ?
C11 C6 C7 C8 -0.3(6) . . . . ?
N2 C6 C7 C8 179.2(3) . . . . ?
C11 C6 C7 N3 -180.0(3) . . . . ?
N2 C6 C7 N3 -0.5(5) . . . . ?
C19 N3 C7 C8 10.9(6) . . . . ?
Zn1 N3 C7 C8 -169.4(3) . . . . ?
C19 N3 C7 C6 -169.4(4) . . . . ?
Zn1 N3 C7 C6 10.2(4) . . . . ?
C6 C7 C8 C9 1.5(6) . . . . ?
N3 C7 C8 C9 -178.8(4) . . . . ?
C7 C8 C9 C10 -1.3(6) . . . . ?
C8 C9 C10 C11 -0.2(6) . . . . ?
C9 C10 C11 C6 1.4(7) . . . . ?
C7 C6 C11 C10 -1.2(6) . . . . ?
N2 C6 C11 C10 179.4(4) . . . . ?
C6 N2 C12 C13 178.4(4) . . . . ?
Zn1 N2 C12 C13 2.6(6) . . . . ?
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N2 C12 C13 C18 7.5(7) . . . . ?
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C12 C13 C14 C15 178.3(5) . . . . ?
C13 C14 C15 C16 0.1(9) . . . . ?
C14 C15 C16 C17 1.4(9) . . . . ?
C15 C16 C17 C18 -1.7(8) . . . . ?
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Zn1 O1 C18 C13 -24.3(6) . . . . ?
Zn1 O1 C18 C17 157.4(3) . . . . ?
C14 C13 C18 O1 -177.4(4) . . . . ?
C12 C13 C18 O1 3.1(7) . . . . ?
C14 C13 C18 C17 0.9(7) . . . . ?
C12 C13 C18 C17 -178.6(4) . . . . ?
C16 C17 C18 O1 178.9(4) . . . . ?
C26 C17 C18 O1 -2.4(7) . . . . ?
C16 C17 C18 C13 0.5(7) . . . . ?
C26 C17 C18 C13 179.2(5) . . . . ?
C7 N3 C19 C20 179.1(4) . . . . ?
Zn1 N3 C19 C20 -0.5(6) . . . . ?
N3 C19 C20 C25 -178.5(4) . . . . ?
N3 C19 C20 C21 -2.2(7) . . . . ?
Zn1 O2 C21 C20 -4.2(6) . . . . ?
Zn1 O2 C21 C22 175.2(3) . . . . ?
C25 C20 C21 O2 -179.3(4) . . . . ?

C19 C20 C21 O2 4.5(6) . . . . ?
C25 C20 C21 C22 1.3(6) . . . . ?
C19 C20 C21 C22 -174.9(4) . . . . ?
O2 C21 C22 C23 179.4(4) . . . . ?
C20 C21 C22 C23 -1.2(6) . . . . ?
O2 C21 C22 C30 -1.4(6) . . . . ?
C20 C21 C22 C30 178.0(3) . . . . ?
C21 C22 C23 C24 0.1(7) . . . . ?
C30 C22 C23 C24 -179.1(4) . . . . ?
C22 C23 C24 C25 1.0(7) . . . . ?
C23 C24 C25 C20 -0.9(7) . . . . ?
C21 C20 C25 C24 -0.2(7) . . . . ?
C19 C20 C25 C24 176.3(4) . . . . ?
C16 C17 C26 C27 -119.4(5) . . . . ?
C18 C17 C26 C27 61.9(6) . . . . ?
C16 C17 C26 C29 0.7(8) . . . . ?
C18 C17 C26 C29 -177.9(5) . . . . ?
C16 C17 C26 C28 118.5(5) . . . . ?
C18 C17 C26 C28 -60.2(6) . . . . ?
C23 C22 C30 C33 -119.9(5) . . . . ?
C21 C22 C30 C33 60.9(5) . . . . ?
C23 C22 C30 C31 0.3(6) . . . . ?
C21 C22 C30 C31 -179.0(4) . . . . ?
C23 C22 C30 C32 120.2(5) . . . . ?
C21 C22 C30 C32 -59.1(5) . . . . ?
O4 Zn2 O3 C47 158.5(3) . . . . ?
N5 Zn2 O3 C47 4.4(3) . . . . ?
N6 Zn2 O3 C47 57.0(5) . . . . ?
N4 Zn2 O3 C47 -101.3(3) . . . . ?
O3 Zn2 O4 C58 171.9(3) . . . . ?
N5 Zn2 O4 C58 -85.5(4) . . . . ?
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O3 Zn2 N6 C44 -61.2(5) . . . . ?
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C34 P2 C34 C35 -4.9(4) 2_655 . . . ?
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C34 P2 C34 C38 168.6(3) 2_655 . . . ?
C36 N4 C35 C34 0.1(5) . . . . ?
Zn2 N4 C35 C34 -173.2(3) . . . . ?
C38 C34 C35 N4 -0.7(5) . . . . ?
P2 C34 C35 N4 172.9(3) . . . . ?
C35 N4 C36 C37 0.8(6) . . . . ?
Zn2 N4 C36 C37 174.1(3) . . . . ?
N4 C36 C37 C38 -1.1(6) . . . . ?
C36 C37 C38 C34 0.5(6) . . . . ?
C35 C34 C38 C37 0.4(6) . . . . ?
P2 C34 C38 C37 -173.8(3) . . . . ?
C45 N5 C39 C40 -6.5(5) . . . . ?
Zn2 N5 C39 C40 177.2(3) . . . . ?
C45 N5 C39 C44 171.9(3) . . . . ?
Zn2 N5 C39 C44 -4.4(4) . . . . ?
C44 C39 C40 C41 -0.4(6) . . . . ?
N5 C39 C40 C41 178.0(3) . . . . ?
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C40 C41 C42 C43 -0.9(6) . . . . ?
C41 C42 C43 C44 0.0(6) . . . . ?
C42 C43 C44 C39 0.6(6) . . . . ?
C42 C43 C44 N6 -176.1(4) . . . . ?
C40 C39 C44 C43 -0.5(5) . . . . ?
N5 C39 C44 C43 -179.0(3) . . . . ?
C40 C39 C44 N6 176.6(3) . . . . ?
N5 C39 C44 N6 -1.9(5) . . . . ?
C52 N6 C44 C43 -0.1(6) . . . . ?
Zn2 N6 C44 C43 -176.0(3) . . . . ?
C52 N6 C44 C39 -177.0(4) . . . . ?
Zn2 N6 C44 C39 7.1(4) . . . . ?
C39 N5 C45 C46 -174.3(3) . . . . ?
Zn2 N5 C45 C46 1.6(5) . . . . ?
N5 C45 C46 C51 -179.9(4) . . . . ?
N5 C45 C46 C47 4.8(6) . . . . ?
Zn2 O3 C47 C46 -0.2(5) . . . . ?
Zn2 O3 C47 C48 -178.6(3) . . . . ?
C51 C46 C47 O3 179.2(3) . . . . ?
C45 C46 C47 O3 -5.6(6) . . . . ?
C51 C46 C47 C48 -2.3(5) . . . . ?
C45 C46 C47 C48 172.8(3) . . . . ?
O3 C47 C48 C49 179.9(4) . . . . ?
C46 C47 C48 C49 1.4(5) . . . . ?
O3 C47 C48 C59 -0.5(6) . . . . ?
C46 C47 C48 C59 -179.0(4) . . . . ?
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C59 C48 C49 C50 -179.3(4) . . . . ?
C48 C49 C50 C51 -1.2(7) . . . . ?
C49 C50 C51 C46 0.3(6) . . . . ?

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C45 C46 C51 C50 -174.1(4) . . . . ?
C44 N6 C52 C53 175.8(4) . . . . ?
Zn2 N6 C52 C53 -8.7(6) . . . . ?
N6 C52 C53 C54 174.8(4) . . . . ?
N6 C52 C53 C58 -7.5(7) . . . . ?
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C54 C53 C58 C57 0.5(6) . . . . ?
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C56 C57 C58 C53 -0.2(6) . . . . ?
C63 C57 C58 C53 -178.3(4) . . . . ?
C49 C48 C59 C61 -1.8(6) . . . . ?
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C49 C48 C59 C62 -120.5(4) . . . . ?
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2 0.000 0.000 0.750 1354.4 144.6
3 0.333 0.667 0.104 342.1 51.5
4 0.333 0.667 0.604 342.1 51.2
5 0.333 0.667 0.358 31.5 2.2

6 0.333 0.667 0.858 31.5 2.2
7 0.667 0.333 0.396 342.1 50.1
8 0.667 0.333 0.896 342.0 49.9
9 0.667 0.333 0.142 31.5 3.0
10 0.667 0.333 0.642 31.5 3.2
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