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to carry out CIF format checking respectively.
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It should be noted that the esd's of the cell dimensions are probably too low;
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Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
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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-
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- **Refine ls goodness of fit ref**: 1.048
- **Refine ls restrained_S all**: 1.142
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- **Refine ls shift/su_mean**: 0.000

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http://www.rsc.org/suppdata/dt/c3/c3dt00078h/c3dt00078h.txt[10-3-2014 11:33:01]
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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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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 $F^2 > 2\sigma(F^2)$ 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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<td>C12</td>
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<td>0.0290 0.8905 -0.1660 0.030 Uiso 1 1 calc R</td>
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<td>C14</td>
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<td>C15</td>
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<td>0.1042 0.8824 -0.1049 0.027 Uiso 1 1 calc R</td>
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<td>H16</td>
<td>H</td>
<td>0.3214(2) 0.92148(13) 0.00702(19) 0.0173(10)</td>
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<td>H17</td>
<td>H</td>
<td>0.2901(3) 0.91882(14) -0.0241(2) 0.0217(11)</td>
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<td>H</td>
<td>0.3019 0.9127 -0.0623 0.026 Uiso 1 1 calc R</td>
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<td>H19</td>
<td>H</td>
<td>0.3478 0.92496(14) 0.0004(2) 0.0235(11)</td>
<td>Uani 1 1 d</td>
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C47 C 0.4176(3) 0.87963(19) 0.1761(3) 0.0466(17) Uani 1 1 d . . .
H47A H 0.4406 0.8785 0.2158 0.070 Uiso 1 1 calc R . .
H47B H 0.4580 0.8810 0.1571 0.070 Uiso 1 1 calc R . .
H47C H 0.3866 0.8542 0.1643 0.070 Uiso 1 1 calc R . .
C48 C 0.4164(4) 0.95895(18) 0.1833(3) 0.0432(15) Uani 1 1 d . . .
H48A H 0.3838 0.9841 0.1794 0.065 Uiso 1 1 calc R . .
H48B H 0.4538 0.9628 0.1620 0.065 Uiso 1 1 calc R . .
H48C H 0.4432 0.9549 0.2222 0.065 Uiso 1 1 calc R . .
C49 C -0.2093(2) 0.77933(13) 0.14208(19) 0.0168(10) Uani 1 1 d . . .
C50 C -0.2290(3) 0.77718(14) 0.19274(19) 0.0208(10) Uani 1 1 d . . .
C51 C -0.2844(2) 0.80075(15) 0.2064(2) 0.0208(10) Uani 1 1 d . . .
H51 H -0.2945 0.7979 0.2413 0.025 Uiso 1 1 calc R . .
C52 C -0.3254(3) 0.82912(15) 0.1672(2) 0.0218(11) Uani 1 1 d . . .
C53 C -0.3105(3) 0.83400(14) 0.1174(2) 0.0207(10) Uani 1 1 d . . .
C54 C -0.2526(2) 0.80910(14) 0.1036(2) 0.0195(10) Uani 1 1 d . . .
C55 C -0.2460(2) 0.81422(13) 0.04883(19) 0.0179(10) Uani 1 1 d . . .
C56 C -0.2093(2) 0.77933(13) -0.02789(19) 0.0184(10) Uani 1 1 d . . .
C57 C -0.2290(3) 0.77718(14) -0.0669(2) 0.0233(11) Uani 1 1 d . . .
C58 C -0.2526(2) 0.80910(14) -0.11965(19) 0.0214(11) Uani 1 1 d . . .
C59 C -0.1836(3) 0.80826(15) -0.1350(2) 0.0238(11) Uani 1 1 d . . .
C60 C -0.1778 0.8122 -0.1709 0.029 Uiso 1 1 calc R . .
C61 C -0.1410(3) 0.77654(14) -0.04500(19) 0.0196(10) Uani 1 1 d . . .
C62 C -0.0653(2) 0.71557(14) -0.0230(2) 0.0191(10) Uani 1 1 d . . .
C63 C -0.0526(2) 0.68099(15) 0.0091(2) 0.0200(10) Uani 1 1 d . . .
C64 C 0.0020(3) 0.64944(14) -0.0204(2) 0.0202(10) Uani 1 1 d . . .
C65 C 0.0405(3) 0.61502(15) 0.0056(2) 0.0244(11) Uani 1 1 d . . .
C66 C 0.0506(3) 0.61062(14) 0.0623(2) 0.0206(10) Uani 1 1 d . . .
C67 C 0.0780 0.5866 0.0801 0.025 Uiso 1 1 calc R . .
C68 C 0.0228(3) 0.63925(14) 0.0939(2) 0.0204(10) Uani 1 1 d . . .
C69 C 0.0168(3) 0.67612(14) 0.0667(2) 0.0210(11) Uani 1 1 d . . .
C70 C 0.0311(3) 0.63173(15) 0.1555(2) 0.0250(11) Uani 1 1 d . . .
C71 C 0.0741(3) 0.66896(16) 0.1898(2) 0.0288(12) Uani 1 1 d . . .
C72 C 0.0716(3) 0.67612(14) 0.1758(2) 0.0233(12) Uani 1 1 d . . .
C73 C 0.0814 0.6630 0.1552 0.045 Uiso 1 1 calc R . .
C74 C 0.0765 0.6046 0.1398 0.045 Uiso 1 1 calc R . .
C75 C 0.0764 0.6538 0.1552 0.045 Uiso 1 1 calc R . .
C76 C 0.0764(3) 0.59101(16) 0.1758(2) 0.0323(12) Uani 1 1 d . . .
C77 C 0.0832 0.5879 0.2154 0.048 Uiso 1 1 calc R . .
C78 C 0.1266 0.5927 0.1682 0.048 Uiso 1 1 calc R . .
C79 C 0.0484 0.5665 0.1566 0.048 Uiso 1 1 calc R . .
C80 C 0.0871(3) 0.86250(14) 0.09144(19) 0.0174(10) Uani 1 1 d . . .
C81 C 0.0745 0.8627 0.0508 0.021 Uiso 1 1 calc R . .
H73B H 0.1287 0.8832 0.1053 0.021 Uiso 1 1 calc R . .
C74 C 0.0509(2) 0.78934(14) 0.09221(19) 0.0161(9) Uani 1 1 d . .
H74A H 0.0376 0.7879 0.0516 0.019 Uiso 1 1 calc R . .
H74B H 0.0681 0.7608 0.1066 0.019 Uiso 1 1 calc R . .
C75 C -0.0425(2) 0.84384(13) 0.08263(19) 0.0161(9) Uani 1 1 d . .
H75A H -0.0878 0.8520 0.1017 0.018 Uiso 1 1 calc R . .
H75B H -0.0577 0.8437 0.0485 0.018 Uiso 1 1 calc R . .
C76 C 0.0365(3) 0.88142(14) 0.16983(19) 0.0188(10) Uani 1 1 d . .
H76A H -0.0103 0.8911 0.1816 0.022 Uiso 1 1 calc RD . .
H76B H 0.0755 0.9040 0.1811 0.023 Uiso 1 1 calc RD . .
C77 C 0.1433(3) 0.81902(14) 0.17267(19) 0.0189(10) Uani 1 1 d . .
H77A H 0.1868 0.8390 0.1838 0.023 Uiso 1 1 calc R . .
H77B H 0.1630 0.7903 0.1743 0.023 Uiso 1 1 calc R . .
C78 C -0.0041(3) 0.79727(14) 0.1792(19) 0.0182(10) Uani 1 1 d . .
H78A H 0.0102 0.7677 0.1792 0.022 Uiso 1 1 calc RD . .
H78B H 0.0522 0.8037 0.1801 0.022 Uiso 1 1 calc R . .
O1W O 0.0084 0.9464 0.2542 0.031 Uani 0.25 1 d PU A -1
H1W1 H -0.0053 0.9631 0.2265 0.047 Uiso 0.25 1 d PD B -1
H1W2 H 0.0251 0.9632 0.2816 0.047 Uiso 0.25 1 d PC -1

Zn1 0.0173(3) 0.0195(3) 0.0159(3) 0.0003(2) 0.0037(2) -0.0003(2)
Zn2 0.0189(3) 0.0196(3) 0.0154(3) 0.0004(2) 0.0064(2) 0.0005(2)
Zn3 0.0192(3) 0.0187(3) 0.0139(3) -0.0009(2) 0.0044(2) -0.0002(2)
P1 0.0199(6) 0.0219(6) 0.0128(6) -0.0006(5) 0.0040(5) 0.0000(4)
N1 0.020(2) 0.0189(19) 0.015(2) -0.0012(16) 0.0014(16) 0.0001(14)
N2 0.024(2) 0.0191(19) 0.017(2) -0.0019(16) 0.0070(17) 0.0003(15)
N3 0.0166(19) 0.0219(19) 0.020(2) -0.0049(16) 0.0063(15) 0.0008(15)
N4 0.021(2) 0.023(2) 0.017(2) -0.0018(16) 0.0086(16) -0.0004(15)
N5 0.0193(19) 0.0179(18) 0.014(2) -0.0001(15) 0.0005(15) -0.0006(15)
N6 0.0184(19) 0.0208(19) 0.014(2) 0.0001(16) 0.0052(15) 0.0006(14)
N7 0.0164(19) 0.0186(18) 0.010(2) 0.0003(15) 0.0044(15) -0.0026(14)
N8 0.0201(19) 0.0191(18) 0.009(2) 0.0016(15) 0.0044(15) 0.0007(14)
N9 0.0162(18) 0.0194(18) 0.009(2) -0.0036(15) 0.0035(14) 0.0003(14)
O1 0.0214(17) 0.0213(16) 0.0214(19) 0.0011(13) 0.0065(13) -0.0024(12)
O2 0.0196(16) 0.0313(17) 0.0165(18) 0.0012(14) 0.0061(13) -0.0010(13)
O3 0.0252(17) 0.0207(16) 0.0199(19) 0.0027(13) 0.0054(14) 0.0006(13)
O4 0.0223(16) 0.0173(15) 0.0232(19) 0.0007(14) 0.0048(14) -0.0026(12)
O5 0.0206(16) 0.0221(16) 0.0181(18) 0.0009(13) 0.0078(13) 0.0006(13)
O6 0.0277(17) 0.0202(16) 0.0169(18) -0.0039(13) 0.0103(14) 0.0029(13)
F1 0.0374(17) 0.0477(18) 0.0169(16) -0.0028(13) 0.0096(13) -0.0100(13)
F2 0.0286(15) 0.0412(17) 0.0303(18) -0.0074(14) 0.0072(13) -0.0164(13)
F3 0.0417(17) 0.0338(16) 0.0221(16) -0.0014(13) 0.0008(13) 0.0134(13)
F4 0.063(2) 0.0240(15) 0.037(2) 0.0122(13) 0.0193(16) 0.0111(14)
F5 0.0328(15) 0.0292(14) 0.0181(16) 0.0039(12) 0.0066(12) 0.0048(11)
F6 0.0288(15) 0.0384(16) 0.0305(18) 0.0012(13) 0.0143(13) 0.0088(12)
C1 0.025(2) 0.019(2) 0.020(3) 0.0056(19) 0.0042(3) 0.0003(18)
C2 0.031(3) 0.024(2) 0.013(3) 0.0012(19) 0.0072(2) -0.0002(19)

http://www.rsc.org/suppdata/dt/c3/c3dt00078h/c3dt00078h.txt[10-3-2014 11:33:01]
C3 0.028(3) 0.028(3) 0.015(3) -0.002(2) 0.002(2) -0.001(2)
C4 0.020(2) 0.026(2) 0.026(3) 0.003(2) 0.000(2) -0.0048(19)
C5 0.024(2) 0.024(2) 0.020(3) -0.001(2) 0.006(2) -0.0002(19)
C6 0.021(2) 0.019(2) 0.020(3) 0.0028(19) 0.006(2) -0.0011(17)
C7 0.023(2) 0.016(2) 0.023(3) 0.0001(19) 0.010(2) 0.0007(17)
C8 0.020(2) 0.018(2) 0.017(3) 0.0021(19) 0.0091(19) 0.0032(17)
C9 0.025(2) 0.021(2) 0.018(3) 0.0021(19) 0.0032(18)
C10 0.027(3) 0.025(2) 0.026(3) 0.003(2) 0.011(2) 0.0039(19)
C11 0.030(3) 0.023(2) 0.018(3) -0.003(2) 0.003(2) 0.0010(19)
C12 0.025(2) 0.025(2) 0.018(3) 0.000(2) 0.005(2) -0.0011(18)
C13 0.021(2) 0.019(2) 0.024(3) 0.007(2) 0.010(2) 0.0002(18)
C14 0.026(3) 0.016(2) 0.014(3) -0.0003(18) 0.004(2) -0.0004(17)
C15 0.016(2) 0.017(2) 0.017(3) 0.0035(18) 0.0017(19) -0.0017(16)
C57 0.027(3) 0.019(2) 0.018(3) -0.0027(19) -0.003(2) -0.0008(18)
C58 0.025(3) 0.021(2) 0.016(3) 0.0052(19) -0.003(2) -0.0008(18)
C59 0.030(3) 0.024(2) 0.017(3) -0.004(2) 0.005(2) -0.0086(19)
C60 0.023(2) 0.025(2) 0.018(3) -0.002(2) 0.008(2) -0.0030(18)
C61 0.023(2) 0.019(2) 0.015(3) -0.0013(18) 0.0032(19) -0.0055(17)
C62 0.019(2) 0.022(2) 0.016(3) -0.0038(19) 0.0041(18) -0.0061(18)
C63 0.017(2) 0.023(2) 0.019(3) -0.0032(19) 0.0033(19) -0.0011(17)
C64 0.024(2) 0.022(2) 0.016(3) -0.0034(19) 0.0074(19) -0.0042(18)
C65 0.020(2) 0.025(2) 0.028(3) -0.007(2) 0.006(2) -0.0028(18)
C66 0.023(2) 0.019(2) 0.021(3) -0.0004(19) 0.008(2) 0.0013(17)
C67 0.017(2) 0.023(2) 0.022(3) 0.001(2) 0.0059(19) 0.0009(17)
C68 0.018(2) 0.023(2) 0.021(3) -0.002(2) 0.0051(19) -0.0048(18)
C69 0.030(3) 0.026(2) 0.019(3) 0.002(2) 0.007(2) 0.006(2)
C70 0.032(3) 0.035(3) 0.019(3) 0.000(2) 0.006(2) 0.007(2)
C71 0.033(3) 0.033(3) 0.026(3) 0.000(2) 0.012(2) 0.001(2)
C72 0.044(3) 0.031(3) 0.021(3) 0.003(2) 0.008(2) 0.006(2)
C73 0.019(2) 0.020(2) 0.013(2) 0.0016(18) 0.0044(18) 0.0011(17)
C74 0.021(2) 0.019(2) 0.010(2) -0.0016(18) 0.0086(18) 0.0009(17)
C75 0.014(2) 0.016(2) 0.017(3) 0.0004(18) 0.0061(18) -0.0028(16)
C76 0.023(2) 0.022(2) 0.011(2) -0.0030(18) 0.0042(18) 0.0000(18)
C77 0.024(2) 0.022(2) 0.010(2) 0.0020(18) 0.0019(18) -0.0001(18)
C78 0.024(2) 0.019(2) 0.013(3) 0.0022(18) 0.0068(19) -0.0010(17)
O1W 0.036 0.033 0.026 0.006 0.012 0.001

_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.

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Zn1 O2 1.976(3) . ?
Zn1 N2 2.071(4) . ?
Zn1 N1 2.107(4) . ?
Zn1 N7 2.194(4) . ?
Zn1 O4 1.960(3) . ?
Zn2 O3 1.966(3) . ?
Zn2 N4 2.082(4) . ?
Zn2 N3 2.111(4) . ?
Zn2 N8 2.201(4) . ?
Zn2 O5 1.959(3) . ?
Zn3 O6 1.969(3) . ?
Zn3 N6 2.071(4) . ?
Zn3 N5 2.123(4) . ?
Zn3 N9 2.200(3) . ?
P1 C76 1.845(5) . ?
P1 C77 1.845(5) . ?
P1 C78 1.853(4) . ?
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N2 C14 1.293(6) . ?
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N7 C76 1.495(6) . ?
N8 C74 1.481(6) . ?
N8 C73 1.484(5) . ?
N8 C77 1.490(6) . ?
N9 C74 1.473(6) . ?
N9 C75 1.479(5) . ?
N9 C78 1.499(6) . ?
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O2 C20 1.309(5) . ?
O3 C25 1.296(6) . ?
O4 C44 1.296(6) . ?
O5 C49 1.295(6) . ?
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F1 C2 1.359(6) . ?
F2 C4 1.372(5) . ?
F3 C26 1.353(6) . ?
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F6 C52 1.357(6) . ?
C1 C2 1.413(7) . ?
C1 C6 1.425(7) . ?
C2 C3 1.361(7) . ?
C3 C4 1.405(8) . ?
C4 C5 1.344(7) . ?
C5 C6 1.427(6) . ?
C6 C7 1.425(7) . ?
C8 C9 1.399(7) . ?
C8 C13 1.413(6) . ?
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C12 C13 1.388(7) . ?
C14 C15 1.429(7) . ?
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C17 C18 1.412(7) . ?
C18 C19 1.363(7) . ?
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O1 Zn1 N2 159.16(14) . . ?
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N2 Zn1 N1 78.93(15) . . ?
O1 Zn1 N7 99.31(13) . . ?
O2 Zn1 N7 96.47(14) . . ?
N2 Zn1 N7 100.39(14) . . ?
N1 Zn1 N7 103.76(14) . . ?
O4 Zn2 O3 97.03(13) . . ?
O4 Zn2 N4 88.79(14) . . ?
O3 Zn2 N4 159.89(15) . . ?
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N4 Zn2 N3 78.41(15) . . ?
O4 Zn2 N8 95.14(14) . . ?
O3 Zn2 N8 98.64(14) . . ?
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N3 Zn2 N8 104.39(14) . . ?
O5 Zn3 O6 97.43(13) . . ?
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N5 Zn3 N9 103.24(13) . . ?
C76 P1 C77 96.4(2) . . ?
C76 P1 C78 96.4(2) . . ?
C77 P1 C78 96.0(2) . . ?
C7 N1 C8 121.5(4) . . ?
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C8 N1 Zn1 113.6(3) . . ?
C14 N2 C13 119.8(4) . . ?
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C13 N2 Zn1 113.8(3) . . ?
C31 N3 C32 121.0(4) . . ?
C31 N3 Zn2 124.4(3) . . ?
C32 N3 Zn2 114.2(3) . . ?
C38 N4 C37 120.8(4) . . ?
C38 N4 Zn2 124.8(3) . . ?
C37 N4 Zn2 113.6(3) . . ?
C55 N5 C56 122.1(4) . . ?
C55 N5 Zn3 124.0(3) . . ?
C56 N5 Zn3 113.4(3) . . ?
C62 N6 C61 119.1(4) . . ?
C62 N6 Zn3 124.7(3) . . ?
C61 N6 Zn3 115.0(3) . . ?
C73 N7 C75 108.5(3) . . ?
C73 N7 C76 111.7(3) . . ?
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C74 N8 C73 108.2(3) . . ?
C74 N8 C77 111.1(3) . . ?
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C74 N8 Zn2 110.8(3) . . ?
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C77 N8 Zn2 106.3(3) . . ?
C74 N9 C75 108.8(3) . . ?
C74 N9 C78 111.1(3) . . ?
C75 N9 C78 111.9(3) . . ?
C74 N9 Zn3 108.5(3) . . ?
C75 N9 Zn3 110.0(2) . . ?
C78 N9 Zn3 106.4(3) . . ?
C1 O1 Zn1 128.3(3) . . ?
C20 O2 Zn1 130.9(3) . . ?
C25 O3 Zn2 129.0(3) . . ?
C44 O4 Zn2 132.2(3) . . ?
C49 O5 Zn3 128.6(3) . . ?
C68 O6 Zn3 132.5(3) . . ?
O1 C1 C2 118.7(5) . . ?
O1 C1 C6 125.9(4) . . ?
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Zn1 O1 C1 C2 -177.2(3) . . . ?
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O1 C1 C2 C3 178.8(4) . . . ?
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'x+1/2, y+1/2, z'
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'x+1/2, -y+1/2, z-1/2'
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_cell_volume 12223.7(14)
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;
SADABS Version 2008/1 Bruker-Nonius
It should be noted that the esd's of the cell dimensions are probably too low; they should be multiplied by a factor of 2 to 10.

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- diffrn_source 'Micorfocus source E025 IuS'
- diffrn_source_type 'Bruker APEX DUO'
- diffrn_source_power  50
- diffrn_source_current  0.6
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- diffrn_radiation_monochromator 'Quazar MX Multilayer Optics'
- diffrn_detector_type '4K CCD area detector APEX II'
- diffrn_measurement_device_type 'APEX DUO Kappa 4-axis goniometer'
- diffrn_measurement_method Fullsphere data collection, phi and omega scans

- diffrn_detector_area_resol_mean 512
- diffrn_reflns_number  211665
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- diffrn_reflns_av_sigmaI/netI 0.0229
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- diffrn_reflns_limit_h_max  40
- diffrn_reflns_limit_k_min  -18
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- diffrn_reflns_limit_l_min  -39
- diffrn_reflns_limit_l_max  39
- diffrn_reflns_theta_min  1.35
- diffrn_reflns_theta_max  28.20
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- reflns_number_gt  12760
- reflns_threshold_expression >2sigma(I)
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- computing_cell_refinement 'Bruker APEX2 v2011.4-0'
- computing_data_reduction 'Bruker SAINT V7.60A'
- computing_structure_solution Sir2011
- computing_structure_refinement 'SHELXS-97 (Sheldrick, 2008)'
- computing_molecular_graphics 'Bruker SHELXTL'
- computing_publication_material 'Bruker SHELXTL'
- refine_special_details

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 $F^2 > 2\sigma(F^2)$ 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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\[ w = 1/\left( s^2 (F_o^2) + (0.0266P)^2 + 22.9438P \right) \]
where \( P = (F_o^2 + 2F_c^2)/3 \)
atom_sites_solution_primary direct
atom_sites_solution_secondary difmap
atom_sites_solution_hydrogens geom
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refine_ls_extinction_coef ?
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refine_ls_number_parameters 855
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refine_ls_goodness_of_fit_ref 1.060
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refine_ls_shift/su_mean 0.000

Zn1 Zn 0.891776(6) 0.947604(15) 0.505822(6) 0.01495(5) Uani 1 1 d . . .
Zn2 Zn 0.914352(6) 0.815517(14) 0.693561(6) 0.01366(5) Uani 1 1 d . . .
Cl1 Cl 0.83001(2) 1.42749(4) 0.54321(2) 0.04877(16) Uani 1 1 d . . .
Cl2 Cl 0.92621(2) 1.40912(4) 0.605325(19) 0.03540(12) Uani 1 1 d . . .
Cl3 Cl 1.103982(14) 0.60653(3) 0.643225(15) 0.02239(9) Uani 1 1 d . . .
Cl4 Cl 1.053918(16) 1.042355(3) 0.67354(2) 0.03329(12) Uani 1 1 d . . .
N1 N 0.85012(5) 1.06944(11) 0.49062(5) 0.0197(3) Uani 1 1 d . . .
N2 N 0.92984(5) 1.05421(10) 0.54406(5) 0.0160(3) Uani 1 1 d . A .
N3 N 0.97814(5) 0.82281(10) 0.68157(5) 0.0153(3) Uani 1 1 d . . .
N4 N 0.93554(5) 0.66940(10) 0.70539(5) 0.0154(3) Uani 1 1 d . A .
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O2 O 0.94188(4) 0.85428(9) 0.51992(4) 0.0167(2) Uani 1 1 d . . .
O3 O 0.91095(4) 0.96109(9) 0.69078(4) 0.0172(2) Uani 1 1 d . . .
O4 O 0.87727(4) 0.79577(9) 0.73871(4) 0.0171(2) Uani 1 1 d . . .
C1 C 0.82769(6) 0.9170(5) 0.41908(6) 0.0231(4) Uani 1 1 d . . .
C2 C 0.81334(7) 0.84815(17) 0.37975(6) 0.0287(5) Uani 1 1 d . . .
C3 C 0.77340(7) 0.86917(19) 0.35100(7) 0.0376(6) Uani 1 1 d . . .
H3 H 0.7638 0.8283 0.3250 0.045 Uiso 1 1 calc R A .
C 4 C 0.74643(7) 0.94748(19) 0.35821(8) 0.0426(6) Uani 1 1 d . . .
H 4 H 0.7185 0.9574 0.3382 0.051 Uiso 1 1 calc R . .
C 5 C 0.80110(6) 0.99444(15) 0.42523(6) 0.0254(4) Uani 1 1 d . . .
H 5 H 0.7678 0.9574 0.3482 0.046 Uiso 1 1 calc R A .
C 6 C 0.81463(6) 1.07060(15) 0.45839(7) 0.0245(4) Uani 1 1 d . . .
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C 7 C 0.86460(6) 1.15213(14) 0.51847(6) 0.0254(4) Uani 1 1 d . . .
C 8 C 0.84086(7) 1.23948(15) 0.51906(7) 0.0285(4) Uani 1 1 d . . .
H 8 H 0.8117 1.2448 0.5012 0.034 Uiso 1 1 calc R . .
C 9 C 0.85935(7) 1.31824(15) 0.54641(6) 0.0185(3) Uani 1 1 d . A .
C 10 C 0.90744(6) 1.14421(13) 0.54641(6) 0.0185(3) Uani 1 1 d . . .
H 10 H 0.9875 1.1060 0.5703 0.020 Uiso 1 1 calc R A .
C 11 C 0.97261(6) 1.04779(13) 0.57529(6) 0.0186(3) Uani 1 1 d . . .
H 11 H 1.0558 1.0380 0.5879 0.022 Uiso 1 1 calc R . .
C 12 C 1.01508(6) 0.79081(12) 0.53794(6) 0.0155(3) Uani 1 1 d . . .
C 13 C 0.98350(5) 0.86943(12) 0.53744(5) 0.0141(3) Uani 1 1 d . . .
H 13 H 0.9498 0.7407 0.4661 0.034 Uiso 1 1 calc R . .
C 14 C 0.96859(6) 0.64375(13) 0.54841(6) 0.0220(4) Uani 1 1 d . . .
H 14 H 0.9432 0.6875 0.5478 0.033 Uiso 1 1 calc R . .
C 15 C 0.90149(7) 1.31013(14) 0.57300(7) 0.0266(4) Uani 1 1 d . . .
C 16 C 0.82221(9) 0.7060(2) 0.32655(8) 0.0546(8) Uani 1 1 d . . .
C 17 C 1.03867(6) 0.61770(19) 0.36574(7) 0.0389(6) Uani 1 1 d . . .
H 17 H 1.0598 0.6463 0.5042 0.037 Uiso 1 1 calc R . .
C 18 C 1.0278 0.5546 0.5071 0.037 Uiso 1 1 calc R .
H 18 H 0.9581 0.5792 0.5361 0.033 Uiso 1 1 calc R .
C 19 C 0.8945(6) 0.68851(13) 0.51914(6) 0.0187(3) Uani 1 1 d . . .
C 20 C 0.96859(6) 0.64375(13) 0.54841(6) 0.0220(4) Uani 1 1 d . . .
H 20 H 0.9432 0.6875 0.5478 0.033 Uiso 1 1 calc R .
C 21 C 0.97476(6) 0.69474(14) 0.46894(6) 0.0226(4) Uani 1 1 d . . .
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C 22 C 0.99945(6) 0.68851(13) 0.51914(6) 0.0187(3) Uani 1 1 d . . .
C 23 C 0.96859(6) 0.64375(13) 0.54841(6) 0.0220(4) Uani 1 1 d . . .
H 23 H 0.9432 0.6875 0.5478 0.033 Uiso 1 1 calc R .
C 24 C 0.97476(6) 0.69474(14) 0.46894(6) 0.0226(4) Uani 1 1 d . . .
H 24 H 0.9498 0.7407 0.4664 0.034 Uiso 1 1 calc R .
C 25 C 0.99945(6) 0.68851(13) 0.51914(6) 0.0187(3) Uani 1 1 d . . .
C 26 C 0.96859(6) 0.64375(13) 0.54841(6) 0.0220(4) Uani 1 1 d . . .
C31 C 0.96313(6) 1.19923(13) 0.69027(6) 0.0219(4) Uani 1 1 d . . .
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C32 C 1.00599(6) 1.17385(14) 0.68497(7) 0.0242(4) Uani 1 1 d . . .
H32 H 1.0274 1.2235 0.6836 0.029 Uiso 1 1 calc R .
C33 C 1.01638(6) 1.07692(14) 0.68185(6) 0.0213(4) Uani 1 1 d . . .
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C34 C 0.98478(6) 1.00230(12) 0.68362(6) 0.0165(3) Uani 1 1 d . . .
C35 C 1.00043(6) 0.90391(13) 0.68109(6) 0.0177(3) Uani 1 1 d . . .
H35 H 1.0306 0.8969 0.6788 0.021 Uiso 1 1 calc R A .
C36 C 0.99845(5) 0.73012(12) 0.67892(6) 0.0155(3) Uani 1 1 d . . .
C37 C 1.03801(6) 0.71592(13) 0.66394(6) 0.0171(3) Uani 1 1 d . . .
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C40 C 0.99322(6) 0.55382(13) 0.68940(6) 0.0192(3) Uani 1 1 d . . .
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 Gobierno Special Details

http://www.rsc.org/suppdata/dt/c3/c3dt00078h/c3dt00078h.txt[10-3-2014 11:33:01]
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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It should be noted that the esd's of the cell dimensions are probably too low;
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F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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H78D H 0.5095 -0.0441 0.3047 0.052 Uiso 0.40 1 calc PR B 2
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C80" C 0.4189(4) 0.0610(9) 0.3173(2) 0.023(3) Uani 0.40 1 d PD B 2
O6" O 0.3797(5) 0.0898(13) 0.2973(3) 0.023(3) Uani 0.40 1 d PD B 2
C81" C 0.4370(2) 0.0094(5) 0.2498(2) 0.030(3) Uani 0.40 1 d PD B 2
C83" C 0.3908(3) -0.0334(7) 0.2365(4) 0.055(4) Uani 0.40 1 d PD B 2
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H83K H 0.3839 -0.0372 0.2068 0.083 Uiso 0.40 1 calc PR B 2
H83L H 0.3659 -0.0041 0.2459 0.083 Uiso 0.40 1 calc PR B 2
C82" C 0.4330(5) 0.0934(6) 0.2305(4) 0.044(4) Uani 0.40 1 d PD B 2
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H82L H 0.4630 0.1204 0.2375 0.066 Uiso 0.40 1 calc PR B 2
C84" C 0.4746(3) -0.0368(7) 0.2333(4) 0.052(4) Uani 0.40 1 d PD B 2
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H85D H 0.4059 0.4038 0.2380 0.026 Uiso 1 1 calc R . .
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H89C H 0.3114 0.3188 0.3343 0.023 Uiso 1 1 calc R B .
H89D H 0.2746 0.3034 0.2934 0.023 Uiso 1 1 calc R . .
C90B C 0.30562(14) 0.3991(2) 0.24417(11) 0.0213(8) Uani 1 1 d . . .
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H1S1 H 0.8567 0.2933 0.6262 0.079 Uiso 0.50 1 calc PR C 1
H1S2 H 0.8509 0.3367 0.6674 0.079 Uiso 0.50 1 calc PR C 1
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C1S2 Cl 0.87445(10) 0.42390(16) 0.62340(9) 0.0604(7) Uani 0.50 1 d P C 1
C1T C 0.0018(6) 0.4543(15) 0.6469(7) 0.168(11) Uani 0.50 1 d P . .
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H1T2 H -0.0236 0.4450 0.6234 0.201 Uiso 0.50 1 calc PR . .
C1T1 Cl 0.05395(15) 0.4159(2) 0.63706(11) 0.0919(12) Uani 0.50 1 d P . .
C1T2 Cl 0.01015(12) 0.5594(2) 0.65583(11) 0.0838(10) Uani 0.50 1 d P . .
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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)
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C58B C57B C62B C61B -1.8(5) ....?
O5B C57B C62B C67B -3.9(5) ....?
C58B C57B C62B C67B 174.8(3) ....?
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C59B C58B C63B C65B -113.6(4) ....?
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C57B C58B C63B C64B -55.4(5) ....?
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C57B C62B C67B N5B 1.8(6) ....?
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C62B C67B N5B C68B -175.0(8) ....?
C62B C67B N5B Zn3B 7.7(5) ....?
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C80B C75B C76B C77B 1.3(13) . . . . ?
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C75B C76B C77B C78B 0.0(14) . . . . ?
C76B C77B C78B C79B -3.1(15) . . . . ?
C77B C78B C79B C80B 4.7(14) . . . . ?
C77B C78B C79B C81B -175.7(8) . . . . ?
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C81B C79B C80B O6B -2.6(15) . . . . ?
C78B C79B C80B C75B -3.4(13) . . . . ?
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C78B C79B C81B C82B -122.2(8) . . . . ?
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N6B - Zn3B - N6 - C73 - 12(4) . . .
N8B - Zn3B - N6 - C73 - 91.8(14) . . .
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C80 - C75 - C77 - C69 - 0(2) . . .
C74 - C75 - C77 - C76 - 178.6(15) . . .
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C76 - C78 - C79 - C80 - 2.6(19) . . .
C76 - C78 - C79 - C81 - -176.7(11) . . .
C77 - C75 - C80 - O6 - 174.1(18) . . .
C74 - C75 - C80 - O6 - -5(3) . . .
C77 - C75 - C80 - C79 - -2(3) . . .
C74 - C75 - C80 - C79 - 179.7(14) . . .
C78 - C79 - C80 - O6 - -175.5(17) . . .
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C78 - C79 - C80 - C75 - 0(2) . . .
C81 - C79 - C80 - C75 - 179.8(13) . . .
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N8B Zn3B O6" C80" 115(2) . . . . ?
C78" C79" C81" C83" -117.9(11) . . . . ?
C80" C79" C81" C83" -61.4(13) . . . . ?
C78" C79" C81" C84" -2.6(12) . . . . ?
C80" C79" C81" C84" 178.1(12) . . . . ?
C78" C79" C81" C82" -122.5(10) . . . . ?
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Zn1B N7B C85B P1B -177.82(16) . . . . ?
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Zn1B N7B C86B N8B 175.5(2) . . . . ?
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SADABS Version 2008/1 Bruker-Nonius
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It should be noted that the esd's of the cell dimensions are probably too low;
they should be multiplied by a factor of 2 to 10
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Fullsphere data collection, phi and omega scans
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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 
\( F^2 > 2\sigma(F^2) \) 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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N3  N  0.22832(18) 1.1050(2) 0.44975(10) 0.0210(7) Uani 1 1 d . . .  
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O2  O  0.36630(15) 0.60674(16) 0.37227(8) 0.0236(6) Uani 1 1 d . . .  
O3  O  0.25071(15) 1.07303(16) 0.54569(8) 0.0226(6) Uani 1 1 d . . .  
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C3 C 0.0810(2) 0.8309(3) 0.27779(13) 0.0283(9) Uani 1 1 d...
H3 H 0.0740 0.8592 0.2487 0.034 Uiso 1 1 calc R B.
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H7 H 0.0458 0.6629 0.4889 0.025 Uiso 1 1 calc R B.
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H8 H 0.0458 0.6629 0.4889 0.025 Uiso 1 1 calc R B.
C9 C 0.1561(2) 0.6188(2) 0.46894(11) 0.0176(8) Uani 1 1 d...
H9 H 0.1561(2) 0.6188(2) 0.46894(11) 0.0176(8) Uani 1 1 d...
C10 C 0.0878(2) 0.5726(2) 0.53597(12) 0.0217(8) Uani 1 1 d...
H10 H 0.0418 0.5767 0.5543 0.026 Uiso 1 1 calc R B.
C11 C 0.1513(2) 0.5151(2) 0.54926(11) 0.0170(7) Uani 1 1 d...
C12 C 0.2184(2) 0.5118(2) 0.52208(11) 0.0183(8) Uani 1 1 d...
H12 H 0.2629 0.4738 0.5308 0.022 Uiso 1 1 calc R B.
C13 C 0.2220(2) 0.5629(2) 0.48601(12) 0.0190(8) Uani 1 1 d...
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C16 C 0.4854(2) 0.4523(3) 0.44596(13) 0.0257(9) Uani 1 1 d...
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C18 C 0.5466(2) 0.4710(3) 0.37448(14) 0.0319(10) Uani 1 1 d...
C19 C 0.5906 0.4579 0.3557 0.038 Uiso 1 1 calc R B.
C20 C 0.5235(2) 0.35640(12) 0.0232(8) Uani 1 1 d...
C21 C 0.4203(2) 0.35640(12) 0.0232(8) Uani 1 1 d...
C22 C 0.2349(2) 0.8293(3) 0.26692(13) 0.0293(9) Uani 1 1 d...
C23 C 0.2958(2) 0.8293(3) 0.26692(13) 0.0293(9) Uani 1 1 d...
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H22B H 0.3414 0.9028 0.2778 0.052 Uiso 1 1 calc R B.
H22C H 0.3167 0.8510 0.3230 0.052 Uiso 1 1 calc R B.
C24 C 0.2121(2) 0.8830(3) 0.22319(13) 0.0372(10) Uani 1 1 d...
H24A H 0.1724 0.8497 0.2035 0.056 Uiso 1 1 calc R B.
H24B H 0.2615 0.8939 0.2065 0.056 Uiso 1 1 calc R B.
H24C H 0.1880 0.9397 0.2317 0.056 Uiso 1 1 calc R B.
C25 C 0.1505(2) 0.4566(2) 0.59233(11) 0.0200(8) Uani 1 1 d...
C26 C 0.0764(2) 0.4751(3) 0.62055(13) 0.0302(10) Uani 1 1 d...
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H26B H 0.0781 0.4362 0.6475 0.045 Uiso 1 1 calc R B.
H26C H 0.0259 0.4641 0.6016 0.045 Uiso 1 1 calc R B.
C27 C 0.2285(2) 0.4728(3) 0.62287(12) 0.0299(9) Uani 1 1 d...
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H27B H 0.2276 0.4359 0.6505 0.045 Uiso 1 1 calc R B.
H27C H 0.2313 0.5354 0.6318 0.045 Uiso 1 1 calc R B.
C28 C 0.1477(2) 0.3592(2) 0.57721(13) 0.0251(9) Uani 1 1 d...
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H67B  H  0.4502  0.7552  0.4180  0.023 Uiso 0.85 1 calc PDU B 1
C68  C  0.3369(2)  0.8428(3)  0.45041(14)  0.0144(7) Uani 0.85 1 d PDU B 1
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H68B  H  0.3213  0.7139  0.5073  0.020 Uiso 0.85 1 calc PDU B 1
C65' C  0.4880(6)  0.8868(9)  0.4687(4)  0.0240(3) Uani 0.15 1 d PDU B 2
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H65D  H  0.5332  0.8512  0.4570  0.029 Uiso 0.15 1 calc PDU B 2
C66' C  0.3919(7)  0.7400(6)  0.4849(3)  0.0189(9) Uani 0.15 1 d PDU B 2
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H2S2  H  0.7944  0.5277  0.6640  0.087 Uiso 0.75 1 calc PDU C 1
C1S' C  0.9033(14)  0.5001(17)  0.7025(9)  0.0480(11) Uani 0.25 1 d PDU D 2
C2S  C  0.8498(4)  0.5127(6)  0.6555(2)  0.0579(18) Uani 0.75 1 d PDU C 1
H2S1' H  0.8936  0.3841  0.7246  0.110 Uiso 0.75 1 calc PR C 1
H2S2' H  0.8248  0.4507  0.7408  0.110 Uiso 0.75 1 calc PDU C 1
C3S  C  0.8229(5)  0.4446(6)  0.7348(3)  0.0736(17) Uani 0.75 1 d PDU C 1
H2S4' H  0.9567  0.5879  0.6572  0.076 Uiso 0.25 1 Calc PR D 2
H2S5' H  0.8230  0.6323  0.6611  0.088 Uiso 0.25 1 calc PDU D 2
C3S' C  0.9659(16)  0.5723(17)  0.6897(10)  0.051(3) Uani 0.25 1 d PDU D 2
H2S6' H  0.8401  0.5304  0.6433  0.088 Uiso 0.25 1 calc PR D 2
H2S7' H  0.7833  0.5156  0.6855  0.088 Uiso 0.25 1 calc PDU D 2
C2S' C  0.8316(12)  0.4941(19)  0.6705(7)  0.059(3) Uani 0.25 1 d PDU D 2
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H2S5' H  0.7833  0.5156  0.6855  0.088 Uiso 0.25 1 calc PDU D 2
http://www.rsc.org/suppdata/dt/c3/c3dt00078h/c3dt00078h.txt[10-3-2014 11:33:01]
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http://www.rsc.org/suppdata/dt/c3/c3dt00078h/c3dt00078h.txt[10-3-2014 11:33:01]
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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Zn1 N1 2.063(3) . ?
Zn1 N2 2.089(3) . ?
Zn1 N5 2.175(3) . ?

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N7 0.0095(13) 0.0172(15) 0.0250(14) -0.0028(12) 0.0015(12) 0.0001(12)
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C67 0.0135(16) 0.0168(17) 0.0250(14) -0.0028(12) 0.0015(12) 0.0001(12)
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_geom_special_details

http://www.rsc.org/suppdata/dt/c3/c3dt00078h/c3dt00078h.txt[10-3-2014 11:33:01]
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N\(\text{C}_46\) 1.292(5) . ?
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<tr>
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<td>C40-C41</td>
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<td>C42</td>
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<tr>
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O3 Zn2 N6 C66 -70.5(2) . . . . ?
O4 Zn2 N6 C66 -168.7(2) . . . . ?
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N3 Zn2 N6 C66 20.5(3) . . . . ?
O3 Zn2 N6 C69 49.0(2) . . . . ?
O4 Zn2 N6 C69 -49.2(2) . . . . ?
N4 Zn2 N6 C69 -139.1(2) . . . . ?
N3 Zn2 N6 C69 140.0(2) . . . . ?
C70 N7 C65 P1 60.9(4) . . . . ?
C69 N7 C65 P1 -60.6(4) . . . . ?
C66 P1 C65 N7 48.4(3) . . . . ?
C67 P1 C65 N7 -49.4(3) . . . . ?
C68 N6 C66 P1 -60.3(4) . . . . ?
C69 N6 C66 P1 60.1(4) . . . . ?
Zn2 N6 C66 P1 176.18(18) . . . . ?
C65 P1 C66 N6 -49.1(3) . . . . ?
C67 P1 C66 N6 47.6(3) . . . . ?
C68 N5 C67 P1 58.2(4) . . . . ?
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Zn1 N5 C67 P1 176.22(18) . . . . ?
C65 P1 C67 N5 51.0(3) . . . . ?
C66 P1 C67 N5 -46.8(3) . . . . ?
C66 N6 C68 N5 66.3(4) . . . . ?
C69 N6 C68 N5 -55.5(4) . . . . ?
Zn2 N6 C68 N5 -169.1(2) . . . . ?
C70 N5 C68 N6 65.3(4) . . . . ?
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Zn1 N5 C68 N6 176.3(2) . . . . ?
C70 N7 C69 N6 -56.7(4) . . . . ?
C65 N7 C69 N6 66.7(4) . . . . ?
C68 N6 C69 N7 55.8(4) . . . . ?
C66 N6 C69 N7 -66.8(4) . . . . ?
Zn2 N6 C69 N7 172.8(3) . . . . ?
C69 N7 C70 N5 57.2(4) . . . . ?
C65 N7 C70 N5 -65.6(4) . . . . ?
C68 N5 C70 N7 -56.3(4) . . . . ?
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C69' N7' C65' P1' -59.8(8) . . . . ?
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SADABS Version 2008/1 Bruker-Nonius
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# SQUEEZE RESULTS (APPEND TO CIF)
# Note: Data are Listed for all Voids in the P1 Unit Cell
# i.e. Centre of Gravity, Solvent Accessible Volume,
# Recovered number of Electrons in the Void and
# Details about the Squeezed Material
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atom_site_occupancy
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Zn2 Zn -0.02897(3) 0.157831(12) -0.10759(2) 0.02674(12) Uani 1 1 d . . .
N1 N 0.0669(2) 0.16960(9) 0.30065(17) 0.0243(6) Uani 1 1 d . . .
N2 N 0.0779(2) 0.23118(9) 0.19959(16) 0.0258(6) Uani 1 1 d . B .
N3 N -0.02897(3) 0.157831(12) -0.10759(2) 0.02674(12) Uani 1 1 d . . .
N4 N -0.02897(3) 0.157831(12) -0.10759(2) 0.02674(12) Uani 1 1 d . B .
O1 O 0.26830(16) 0.14769(8) 0.33192(14) 0.0273(5) Uani 1 1 d . . .
O2 O 0.25842(17) 0.20019(7) 0.18836(14) 0.0276(5) Uani 1 1 d . . .
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C1 C 0.2570(2) 0.12172(10) 0.38596(19) 0.0230(7) Uani 1 1 d . . .
C2 C 0.3401(2) 0.09645(10) 0.43669(19) 0.0234(7) Uani 1 1 d . . .
C3 C 0.3274(2) 0.06929(11) 0.4945(2) 0.0282(7) Uani 1 1 d . . .
H3 H 0.3832 0.0525 0.5270 0.034 Uiso 1 1 calc R B .
C4 C 0.2384(3) 0.06428(11) 0.5089(2) 0.0289(7) Uani 1 1 d . A .
C5 C 0.1656(2) 0.11718(10) 0.4000(2) 0.0246(7) Uani 1 1 d . . .
C6 C 0.0785(2) 0.14289(11) 0.3596(2) 0.0258(7) Uani 1 1 d . . .
H6 H 0.0244 0.1398 0.3782 0.031 Uiso 1 1 calc R B .
C7 C -0.0187(2) 0.19610(11) 0.2683(2) 0.0254(7) Uani 1 1 d . . .
C8 C -0.1059(3) 0.19102(12) 0.2841(2) 0.0312(8) Uani 1 1 d . . .
H8 H -0.1129 0.1671 0.3159 0.037 Uiso 1 1 calc R . .
C9 C -0.1833(3) 0.22069(14) 0.2537(2) 0.0367(9) Uani 1 1 d . . .
H9 H -0.2418 0.2177 0.2664 0.044 Uiso 1 1 calc R B .
C10 C -0.1748(3) 0.25472(13) 0.2045(2) 0.0402(9) Uani 1 1 d . . .
H10 H -0.2272 0.2752 0.1841 0.048 Uiso 1 1 calc R . .
C11 C -0.0904(3) 0.25868(12) 0.1855(2) 0.0347(8) Uani 1 1 d . . .
H11 H -0.0861 0.2814 0.1503 0.042 Uiso 1 1 calc R B .
C12 C -0.0110(2) 0.22995(11) 0.2169(2) 0.0261(7) Uani 1 1 d . B .
C13 C 0.1029(3) 0.26548(11) 0.1682(2) 0.0293(7) Uani 1 1 d . . .
H13 H 0.0591 0.2896 0.1582 0.035 Uiso 1 1 calc R B .
C14 C 0.1897(3) 0.27052(11) 0.1474(2) 0.0317(8) Uani 1 1 d . . .
C15 C 0.2005(3) 0.31180(12) 0.1151(2) 0.0364(8) Uani 1 1 d . . .
H15 H 0.1497 0.3329 0.1064 0.044 Uiso 1 1 calc R B .
C16 C 0.2817(3) 0.32156(13) 0.0966(2) 0.0412(9) Uani 1 1 d . . .
H16 H 0.2878 0.3492 0.0751 0.049 Uiso 1 1 calc R . .
C17 C 0.3568(3) 0.29027(13) 0.1097(2) 0.0411(9) Uani 1 1 d . . .
H17 H 0.4136 0.2974 0.0966 0.049 Uiso 1 1 calc R B .
C18 C 0.3514(3) 0.24951(12) 0.1410(2) 0.0339(8) Uani 1 1 d . . .
C19 C 0.2647(3) 0.23849(12) 0.1595(2) 0.0299(7) Uani 1 1 d . . .
C20 C 0.4426(2) 0.10154(10) 0.4281(2) 0.0255(7) Uani 1 1 d . . .
C21 C 0.4811(3) 0.14775(11) 0.4543(2) 0.0323(8) Uani 1 1 d . . .
H21 A H 0.4342 0.1688 0.4190 0.048 Uiso 1 1 calc R . .
H21 B H 0.5464 0.1514 0.4493 0.048 Uiso 1 1 calc R .
H21 C H 0.4872 0.1525 0.5112 0.048 Uiso 1 1 calc R .
C22 C 0.4368(3) 0.09293(12) 0.3404(2) 0.0318(8) Uani 1 1 d . . .
H22 A H 0.4135 0.0632 0.3248 0.048 Uiso 1 1 calc R . .
H22B H 0.5030 0.0966 0.3372 0.048 Uiso 1 1 calc R . .
H22C H 0.3903 0.1135 0.3033 0.048 Uiso 1 1 calc R . .
C23 C 0.5192(3) 0.06983(12) 0.4831(2) 0.0329(8) Uani 1 1 d . .
H23A H 0.5230 0.0734 0.5397 0.049 Uiso 1 1 calc R . .
H23B H 0.5846 0.0758 0.4797 0.049 Uiso 1 1 calc R . .
H23C H 0.4992 0.0401 0.5397 0.049 Uiso 1 1 calc R . .
C24 C 0.2298(3) 0.03520(12) 0.5777(2) 0.0379(8) Uani 0.60 1 d PDU A 1
C25 C 0.1395(5) 0.0053(3) 0.5425(6) 0.0481(19) Uani 0.60 1 d PDU A 1
H25A H 0.0795 0.0088 0.5170 0.072 Uiso 0.60 1 calc PR A 1
H25B H 0.1229 -0.0022 0.5571 0.074 Uiso 0.60 1 calc PR A 1
H25C H 0.1008 0.0041 0.5048 0.074 Uiso 0.60 1 calc PR A 1
C26 C 0.2131(6) 0.0632(2) 0.6441(4) 0.0443(16) Uani 0.60 1 d PDU A 1
H26A H 0.2681 0.0838 0.6656 0.066 Uiso 0.60 1 calc PR A 1
H26B H 0.2103 0.0445 0.6885 0.066 Uiso 0.60 1 calc PR A 1
H26C H 0.1502 0.0791 0.6206 0.066 Uiso 0.60 1 calc PR A 1
C27 C 0.3221(5) 0.0075(2) 0.5919(8) 0.050(2) Uani 0.40 1 d PDU A 2
C27' C 0.3013(8) -0.0029(3) 0.5919(8) 0.050(2) Uani 0.40 1 d PDU A 2
C28 C 0.4353(3) 0.21604(14) 0.1546(2) 0.0414(9) Uani 1 1 d . .
C29 C 0.5217(3) 0.23528(18) 0.1335(3) 0.0612(14) Uani 1 1 d . .
H29A H 0.4977 0.2436 0.0756 0.092 Uiso 1 1 calc R . .
H29B H 0.5747 0.2136 0.1439 0.092 Uiso 1 1 calc R . .
H29C H 0.5479 0.2609 0.1674 0.092 Uiso 1 1 calc R . .
C30 C 0.4772(3) 0.20206(16) 0.2446(3) 0.0504(11) Uani 1 1 d . .
H30A H 0.5018 0.2276 0.2793 0.076 Uiso 1 1 calc R . .
H30B H 0.5321 0.1816 0.2529 0.076 Uiso 1 1 calc R . .
H30C H 0.4246 0.1881 0.2590 0.076 Uiso 1 1 calc R . .
C31 C 0.3964(3) 0.17693(15) 0.1546(2) 0.0414(9) Uani 1 1 d . .
C32 C -0.1296(3) 0.22638(10) -0.04731(19) 0.0265(7) Uani 1 1 d . .
C33 C -0.2205(3) 0.24167(11) -0.0385(2) 0.0280(7) Uani 1 1 d . .
C34 C -0.2267(3) 0.28462(11) -0.0213(2) 0.0291(7) Uani 1 1 d . .
H34 H -0.2876 0.29477 -0.0180 0.035 Uiso 1 1 calc RB .
C35 C -0.1493(3) 0.31511(11) -0.0080(2) 0.0281(7) Uani 1 1 d . .
C36 C -0.0636(3) 0.30023(11) -0.0162(2) 0.0271(7) Uani 1 1 d . .
H36 H -0.0099 0.3199 -0.0075 0.033 Uiso 1 1 calc RB .
C37 C -0.0521(2) 0.25691(10) -0.0369(2) 0.0253(7) Uani 1 1 d . .
C38 C 0.0349(3) 0.24834(11) -0.0559(2) 0.0271(7) Uani 1 1 d . .
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<td>Uani 1 1</td>
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<td>-0.0028(4)</td>
<td>0.0388(12)</td>
<td>Uani 0.60 1 d PDU B 1</td>
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<td>0.1769</td>
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<td>0.07129(17)</td>
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<td>0.1472(7)</td>
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<td>0.1681</td>
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<td>0.1049</td>
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http://www.rsc.org/suppdata/dt/c3/c3dt00078h/c3dt00078h.txt[10-3-2014 11:33:01]
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C12X Cl -0.3425(6) 0.3936(3) -0.3000(5) 0.121(3) Uani 0.25 1 d PDU C 1
C1Z C -0.1906(14) 0.4668(5) -0.3277(8) 0.061(3) Uani 0.25 1 d PDU D 2
H1Z1 H -0.2397 0.4874 -0.3206 0.073 Uiso 0.25 1 calc PR D 2
H1Z2 H -0.1364 0.4840 -0.3355 0.073 Uiso 0.25 1 calc PR D 2
C11Z Cl -0.2493(6) 0.4348(3) -0.4163(5) 0.122(3) Uani 0.25 1 d PDU D 2
C1Z1 Zn 0.02120(19) 0.0268(2) 0.0183(2) 0.00253(14) 0.00605(15) 0.00031(14)
C1Z2 Zn 0.0337(2) 0.0255(2) 0.0185(2) -0.00037(14) 0.00626(16) 0.00597(15)
N1 0.0211(13) 0.0297(14) 0.0204(14) 0.0019(11) 0.0054(11) 0.0005(11)
N2 0.0317(15) 0.0266(14) 0.0212(14) 0.0046(11) 0.0105(12) 0.0080(11)
N3 0.0439(17) 0.0330(15) 0.0241(15) 0.0000(12) 0.0100(13) 0.0098(13)
O1 0.0214(11) 0.0349(12) 0.0227(12) 0.0072(10) 0.0044(9) -0.0010(9)
O2 0.0278(12) 0.0311(12) 0.0260(12) 0.0048(10) 0.0122(10) -0.0005(9)
O3 0.0368(13) 0.0242(11) 0.0280(13) 0.0015(11) 0.0128(11) 0.0040(9)
O4 0.0378(14) 0.0317(13) 0.0286(13) -0.0066(11) 0.0015(11) 0.0026(11)
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C4 0.0317(18) 0.0271(16) 0.0302(18) 0.0026(14) 0.0139(15) 0.0012(13)
C5 0.0231(16) 0.0272(16) 0.0222(16) 0.0003(13) 0.0066(13) -0.0006(12)
C6 0.0246(16) 0.0307(16) 0.0223(17) 0.0002(13) 0.0085(13) -0.0028(13)
C7 0.0219(16) 0.0323(17) 0.0189(16) -0.0021(13) 0.0036(13) 0.0034(13)
C8 0.0252(17) 0.0424(19) 0.0250(18) 0.0042(15) 0.0077(14) 0.0025(14)
C9 0.0259(18) 0.058(2) 0.0281(19) 0.0065(17) 0.0113(15) 0.0097(16)
C10 0.0322(19) 0.049(2) 0.038(2) 0.0083(18) 0.0098(17) 0.0164(17)
C11 0.0334(19) 0.0377(19) 0.033(2) 0.0100(16) 0.0123(16) 0.0087(15)
C12 0.0242(16) 0.0323(17) 0.0210(16) -0.0012(13) 0.0072(13) 0.0036(13)
C13 0.0309(17) 0.0258(16) 0.0277(18) 0.0019(14) 0.0062(14) 0.0007(13)
C14 0.0323(18) 0.0330(18) 0.0272(18) 0.0036(14) 0.0076(15) -0.0029(14)
C15 0.042(2) 0.0323(18) 0.034(2) 0.0048(15) 0.0125(17) -0.0025(15)
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C20 0.0203(15) 0.0261(15) 0.0267(17) 0.0002(13) 0.0043(13) -0.0006(12)
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C22 0.0268(17) 0.0407(19) 0.0286(18) -0.0056(15) 0.0108(14) -0.0049(14)
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C24 0.0457(17) 0.0330(16) 0.0393(17) 0.0127(13) 0.0203(14) 0.0042(13)
C25 0.051(3) 0.042(4) 0.048(4) 0.014(3) 0.015(3) -0.005(3)
C26 0.060(4) 0.040(3) 0.037(3) 0.014(2) 0.022(3) 0.013(3)
C27 0.045(3) 0.034(3) 0.041(4) 0.012(3) 0.017(3) 0.002(3)
C24' 0.0457(17) 0.0330(16) 0.0393(17) 0.0127(13) 0.0203(14) 0.0042(13)

http://www.rsc.org/suppdata/dt/c3/c3dt00078h/c3dt00078h.txt[10-3-2014 11:33:01]
C65' 0.040(2) 0.026(2) 0.020(2) 0.005(2) 0.002(2) -0.003(2)
C66' 0.048(2) 0.027(2) 0.022(2) 0.000(2) -0.001(2) -0.002(2)
C67' 0.051(2) 0.031(2) 0.022(2) -0.007(2) 0.002(2) 0.010(2)
C68' 0.042(2) 0.029(2) 0.019(2) 0.003(2) 0.006(2) 0.010(2)
C69' 0.073(3) 0.030(2) 0.027(3) -0.001(2) -0.008(3) 0.006(2)
C70 0.0329(18) 0.0274(16) 0.0283(18) 0.0018(14) 0.0116(15) 0.0013(13)
C1X 0.049(8) 0.033(8) 0.093(14) -0.001(7) 0.016(6) 0.027(6)
C11X 0.0676(18) 0.0488(12) 0.0763(17) -0.0124(12) 0.0560(12) -0.0077(12)
C12X 0.093(5) 0.158(8) 0.095(5) -0.019(5) 0.015(4) -0.073(5)
C1Z 0.060(6) 0.058(5) 0.064(4) -0.021(3) 0.022(4) 0.001(4)
C11Z 0.091(5) 0.172(8) 0.115(4) -0.110(5) 0.050(4) -0.045(5)
C12Z 0.0676(18) 0.0488(12) 0.0763(17) -0.0124(12) 0.0560(12) -0.0077(12)

_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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Zn1 O2 1.974(2).?
Zn1 N2 2.062(3).?
Zn1 N1 2.079(3).?
Zn1 N6' 2.163(8).?
Zn1 N5 2.206(6).?
Zn2 O4 1.953(2).?
Zn2 O3 1.957(2).?
Zn2 N3 2.053(3).?
Zn2 N4 2.071(3).?
Zn2 N6 2.179(6).?
Zn2 N5' 2.189(9).?
N1 C6 1.284(4).?
N1 C7 1.416(4).?
N2 C13 1.301(4).?
N2 C12 1.415(4).?
N3 C38 1.294(4).?
N3 C39 1.417(4).?
N4 C45 1.302(5).?
N4 C44 1.423(5).?
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O2 C19 1.300(4).?
O3 C32 1.301(4).?
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C1 C5 1.427(5).?
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C7 C12 1.408(5) . ?
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C14 C15 1.423(5) . ?
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C17 C18 1.384(5) . ?
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C20 C21 1.538(4) . ?
C24 C27 1.527(6) . ?
C24 C25 1.530(7) . ?
C24 C26 1.534(7) . ?
C28 C31 1.522(7) . ?
C28 C30 1.533(6) . ?
C28 C29 1.536(6) . ?
C32 C37 1.420(5) . ?
C32 C33 1.448(5) . ?
C33 C34 1.368(5) . ?
C33 C52 1.529(5) . ?
C34 C35 1.411(5) . ?
C35 C36 1.369(5) . ?
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C36 C37 1.409(5) . ?
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C46 C51 1.419(5) . ?
C46 C47 1.424(6) . ?
C47 C48 1.444(5) . ?
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C56 C59 1.527(6) . ?
C56 C57 1.546(6) . ?
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C60 C63 1.539(6) . ?
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P1 C67 1.841(4) . ?
P1 C69 1.851(4) . ?
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N5 C66 1.481(4) . ?
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N7 C66 1.485(4) . ?
N7 C65 1.498(5) . ?
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P1' C68' 1.850(5) . ?
P1' C67' 1.866(5) . ?
N5' C64' 1.480(5) . ?
N5' C66' 1.484(5) . ?
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N6' C64' 1.480(5) . ?
N6' C65' 1.481(5) . ?
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C12 N2 Zn1 113.8(2) . . ?
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C10 C11 C12  121.2(3) 
C11 C12 C7   118.9(3) 
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C19 C14 C13  124.9(3) 
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C14 C19 C18  118.4(3) 
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C30 C28 C29  107.6(3) 
C31 C28 C18  110.1(3) 
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O3 C32 C33  119.2(3) 
C37 C32 C33  117.8(3) 
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C65 N6 Zn2 114.3(5) ...?
C69 N7 C66 108.5(5) ...?
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O2 Zn1 N2 C13 -12.6(3) . . . .
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N6' Zn1 N2 C13 -106.0(4) . . . .
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O2 Zn1 N2 C12 175.1(2) . . . .
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O3 Zn2 N3 C38 -3.1(3) . . . .
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N6 Zn2 N3 C38 -97.3(4) . . . .
N5' Zn2 N3 C38 -96.7(5) . . . .
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N5' Zn2 N3 C39 88.0(4) . . . .
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O3 Zn2 N4 C45 -124.1(4) . . . .
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N5' Zn2 N4 C45 80.4(5) . . . .
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