Table 1. CIF1 for the 3:3 p,p-Zn₃L^4–trithiocyanuric acid^{3-} complex (11) (data no. RGK619, registration number CCDC-174993)

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Crystals deposited from concentrated aqueous solution were covered by
powdery crystals. They could not be clean up because of their instability
in air. A number of reflections were overlapped by those of crystallites,
especially in the range of lower 2θ angle. After checking the intensities
of equivalent reflections, the reflections exhibitting a low internal
consistency were removed. The completeness thus was reduced to approximately
0.83. Although 48.5 oxygen atoms of nine nitrate ions and 21.5 water molecules
should be located, only 38.5 atoms involving those of five nitrate ions were found.
A total of 10 oxygen and 4 nitrogen atoms were missing. The atoms of cyclen
rings were refined isotropically, of which hydrogen atoms excluding those
attached to nitrogens were not assigned. The bond lengths of C139-C140,
C140-N141, and N-O of nitrate ions were restrained. These facts seem to result
in considerably large R values.

;
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data_RGK619raplt_Hiroshima_Univ
#---
CHEMICAL DATA
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_chemical_formula_moiety   'C129 H216 N45 S9 Zn9, 21.5(H2 O), 9(N O3)'
_chemical_formula_weight   4219.76
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CRYSTAL DATA
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_cell_length_b          21.438(2)
_cell_length_c          29.380(3)
_cell_angle_alpha        92.417(2)
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_cell_volume            9659(2)
_cell_formula_units_Z       2
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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^, whereas conventional R factors (gt)
 are based on F, with F set to zero for negative F^2^. The threshold
 expression of F^2^ > 2σ(F^2^) is used only for calculating R factor (gt).
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_refine_ls_number_parameters   1369
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_refine_ls_weighting_scheme   calc
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Zn3 Zn 0.73069(8) 0.13167(7) 0.97353(5) 0.0614(4) Uani 1 1 d . . .
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Zn66 Zn 0.76184(9) 0.40932(7) 0.56590(5) 0.0637(4) Uani 1 1 d . . .
Zn67 Zn 0.63341(8) 0.44594(7) 0.94628(5) 0.0576(4) Uani 1 1 d . . .
Zn129 Zn 0.58244(8) 0.20776(7) 0.13932(5) 0.0597(4) Uani 1 1 d . . .
Zn130 Zn 0.45948(8) 0.22429(7) 0.52713(5) 0.0568(4) Uani 1 1 d . . .
Zn131 Zn 0.29223(7) 0.18657(6) 0.90544(5) 0.0515(3) Uani 1 1 d . . .
S62 S 1.0198(2) 0.2748(2) 0.2033(2) 0.088(1) Uani 1 1 d . . .
S63 S 0.7706(3) 0.4081(2) 0.1465(1) 0.083(1) Uani 1 1 d . . .
S64 S 0.7121(2) 0.1623(2) 0.1389(1) 0.0667(9) Uani 1 1 d . . .
S126 S 0.8682(2) 0.2679(2) 0.5882(1) 0.0643(8) Uani 1 1 d . . .
S127 S 0.5740(2) 0.1291(2) 0.5439(1) 0.0661(9) Uani 1 1 d . . .
S128 S 0.5829(2) 0.3742(2) 0.5443(1) 0.0598(8) Uani 1 1 d . . .
S190 S 0.7278(2) 0.2357(2) 0.9958(1) 0.0692(9) Uani 1 1 d . . .
S191 S 0.4990(2) 0.3879(1) 0.9402(1) 0.0550(7) Uani 1 1 d . . .
S192 S 0.4093(2) 0.1437(2) 0.9399(1) 0.0576(8) Uani 1 1 d . . .
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O2W O 0.9514(8) 0.0432(5) 0.3956(4) 0.100(3) Uiso 1 1 d . . .
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O3W O 0.2034(8) 0.2063(5) 0.3844(4) 0.100(3) Uiso 1 1 d . . .
O4W O 0.3679(8) 0.0859(6) 0.3083(4) 0.109(4) Uiso 1 1 d . . .
O5W O 0.3313(8) 0.2056(6) 0.3178(4) 0.104(3) Uiso 1 1 d . . .
O6W O 0.1149(8) 0.1109(6) 0.4316(4) 0.109(4) Uiso 1 1 d . . .
O7W O 0.023(1) 0.2444(7) 0.8204(5) 0.139(5) Uiso 1 1 d . . .
O8W O 0.375(1) 0.3345(8) 0.3182(5) 0.146(5) Uiso 1 1 d . . .
O9W O 0.118(1) 0.2025(8) 0.5036(5) 0.143(5) Uiso 1 1 d . . .
O10W O 0.562(1) 0.475(1) 0.2476(7) 0.183(7) Uiso 1 1 d . . .
O11W O 0.065(1) 0.320(1) 0.5048(7) 0.183(7) Uiso 1 1 d . . .
O12W O 0.196(1) 0.312(1) 0.2940(7) 0.184(7) Uiso 1 1 d . . .
O13W O 0.224(1) 0.406(1) 0.2264(7) 0.191(7) Uiso 1 1 d . . .
O14W O 0.098(1) 0.2042(9) 0.5955(6) 0.168(6) Uiso 1 1 d . . .
O15W O 0.279(2) 0.262(1) 0.1368(7) 0.201(8) Uiso 1 1 d . . .
O16W O 0.155(1) 0.3451(9) 0.1336(7) 0.176(7) Uiso 1 1 d . . .
O17W O 0.396(1) 0.3981(9) 0.2422(6) 0.173(6) Uiso 1 1 d . . .
O18W O 0.714(1) 0.006(1) 0.2734(7) 0.189(7) Uiso 1 1 d . . .
O19W O 0.296(1) 0.009(1) 0.2310(7) 0.178(7) Uiso 1 1 d . . .
O20W O 0.473(1) 0.423(1) 0.3805(7) 0.184(7) Uiso 1 1 d . . .
O21W O 0.427(1) 0.014(1) 0.5241(7) 0.187(7) Uiso 1 1 d . . .
O22W O 0.948(2) 0.296(2) 0.904(1) 0.28(1) Uiso 1 1 d . . .
O23W O 1.004(2) 0.322(2) 0.695(1) 0.29(1) Uiso 1 1 d . . .
O24W O 0.397(2) 0.423(2) 0.678(1) 0.30(2) Uiso 1 1 d . . .
O25W O 0.995(3) 0.195(2) 0.042(1) 0.33(2) Uiso 1 1 d . . .
O202 O 0.0709(9) 0.3461(7) 0.3474(4) 0.132(4) Uiso 1 1 d D . .
O203 O 0.1325(4) 0.3189(6) 0.4132(4) 0.119(4) Uiso 1 1 d D . .
O204 O 0.0464(4) 0.3868(7) 0.4146(5) 0.157(6) Uiso 1 1 d D . .
O206 O 0.1294(3) 0.0918(6) 1.0173(4) 0.106(3) Uiso 1 1 d D . .
O207 O 0.2083(9) 0.1654(5) 1.0525(6) 0.160(6) Uiso 1 1 d D . .
O208 O 0.2246(4) 0.0703(5) 1.0732(3) 0.096(3) Uiso 1 1 d D . .
O210 O 0.7174(2) 0.0001(7) 1.1422(5) 0.130(4) Uiso 1 1 d D . .
O211 O 0.5948(4) 0.0323(5) 1.1180(3) 0.085(3) Uiso 1 1 d D . .
O212 O 0.6236(7) 0.010(1) 1.1899(4) 0.197(8) Uiso 1 1 d D . .
O214 O 0.3210(3) 0.4647(5) 0.8774(3) 0.088(3) Uiso 1 1 d D . .
O215 O 0.4405(4) 0.4934(7) 0.8428(3) 0.129(4) Uiso 1 1 d D . .
O216 O 0.4284(5) 0.5227(4) 0.9118(3) 0.080(3) Uiso 1 1 d D . .
O218 O 0.9606(7) 0.1088(5) 0.8187(4) 0.094(3) Uiso 1 1 d D . .
O219 O 1.0079(3) 0.0882(9) 0.7536(6) 0.164(6) Uiso 1 1 d D . .
O220 O 0.8928(4) 0.0333(9) 0.7744(8) 0.212(9) Uiso 1 1 d D . .
N4 N 0.9776(7) 0.1400(5) 0.2761(4) 0.071(3) Uiso 1 1 d . . .
N7 N 1.1488(9) 0.1617(6) 0.2478(5) 0.091(4) Uiso 1 1 d . . .
N10 N 1.0990(9) 0.1309(7) 0.1563(5) 0.095(4) Uiso 1 1 d . . .
N13 N 0.9270(7) 0.1024(5) 0.1840(4) 0.072(3) Uiso 1 1 d . . .
N16 N 0.8315(6) 0.1174(5) 0.5062(3) 0.057(2) Uiso 1 1 d . . .
N19 N 0.7320(7) 0.0445(5) 0.5679(4) 0.065(3) Uiso 1 1 d . . .
N22 N 0.7830(7) 0.1174(5) 0.6510(3) 0.062(3) Uiso 1 1 d . . .
N25 N 0.9244(7) 0.1157(5) 0.5948(3) 0.064(3) Uiso 1 1 d . . .
N28 N 0.7122(6) 0.1177(5) 0.8958(3) 0.056(2) Uiso 1 1 d . . .
N31 N 0.6176(6) 0.0663(5) 0.9660(3) 0.059(2) Uiso 1 1 d . . .
N34 N 0.7630(7) 0.0765(5) 1.0320(4) 0.068(3) Uiso 1 1 d . . .
N37 N 0.8627(7) 0.1202(5) 0.9611(4) 0.067(3) Uiso 1 1 d . . .

N57 N 0.8896(8) 0.3327(7) 0.1734(4) 0.084(3) Uani 1 1 d . . .
N59 N 0.7511(6) 0.2850(5) 0.1443(3) 0.059(3) Uani 1 1 d . . .
N61 N 0.8648(6) 0.2235(6) 0.1674(3) 0.066(3) Uani 1 1 d . . .
N68 N 0.8718(7) 0.4509(5) 0.2632(3) 0.064(3) Uiso 1 1 d . . .
N71 N 1.0076(7) 0.4520(5) 0.2036(4) 0.074(3) Uiso 1 1 d . . .
N74 N 0.934(1) 0.5413(8) 0.1513(6) 0.125(5) Uiso 1 1 d . . .
N77 N 0.8033(8) 0.5454(6) 0.2152(4) 0.083(3) Uiso 1 1 d . . .
N80 N 0.7998(6) 0.4251(5) 0.4968(3) 0.058(2) Uiso 1 1 d . . .
N83 N 0.8948(7) 0.4212(5) 0.5818(4) 0.069(3) Uiso 1 1 d . . .
N86 N 0.7591(7) 0.4271(5) 0.6394(4) 0.073(3) Uiso 1 1 d . . .
N89 N 0.7279(7) 0.4998(5) 0.5641(4) 0.068(3) Uiso 1 1 d . . .
N92 N 0.6828(8) 0.4305(6) 0.8777(4) 0.082(3) Uiso 1 1 d . . .
N95 N 0.6200(9) 0.5341(6) 0.9203(5) 0.091(4) Uiso 1 1 d . . .
N98 N 0.6712(8) 0.5019(6) 1.0081(4) 0.083(3) Uiso 1 1 d . . .
N101 N 0.7471(9) 0.4061(7) 0.9664(5) 0.093(4) Uiso 1 1 d . . .
N121 N 0.7169(5) 0.2078(4) 0.5659(3) 0.046(2) Uani 1 1 d . . .
N123 N 0.5886(6) 0.2495(4) 0.5449(3) 0.051(2) Uani 1 1 d . . .
N125 N 0.7180(5) 0.3142(4) 0.5617(3) 0.049(2) Uani 1 1 d . . .
N132 N 0.5540(8) 0.2348(6) 0.2099(4) 0.087(3) Uiso 1 1 d . . .
N135 N 0.571(1) 0.3002(7) 0.1318(5) 0.110(4) Uiso 1 1 d . . .
N138 N 0.5033(9) 0.1961(7) 0.0729(5) 0.100(4) Uiso 1 1 d . . .
N141 N 0.4882(3) 0.1324(6) 0.1509(4) 0.091(4) Uiso 1 1 d D . .
N144 N 0.4590(6) 0.2277(5) 0.4519(3) 0.059(2) Uiso 1 1 d . . .
N147 N 0.3678(7) 0.1465(5) 0.5111(3) 0.063(3) Uiso 1 1 d . . .
N150 N 0.4048(7) 0.2226(5) 0.5938(3) 0.060(3) Uiso 1 1 d . . .
N153 N 0.3857(6) 0.3005(5) 0.5196(3) 0.060(3) Uiso 1 1 d . . .
N156 N 0.3114(6) 0.1991(5) 0.8317(3) 0.058(2) Uiso 1 1 d . . .
N159 N 0.2021(6) 0.1121(4) 0.8772(3) 0.053(2) Uiso 1 1 d . . .
N162 N 0.1882(6) 0.1971(5) 0.9514(3) 0.059(2) Uiso 1 1 d . . .
N165 N 0.2897(6) 0.2850(5) 0.9046(3) 0.057(2) Uiso 1 1 d . . .
N185 N 0.6090(5) 0.3057(5) 0.9660(3) 0.053(2) Uani 1 1 d . . .
N187 N 0.4637(5) 0.2666(5) 0.9404(3) 0.052(2) Uani 1 1 d . . .
N189 N 0.5631(5) 0.1966(4) 0.9660(3) 0.053(2) Uani 1 1 d . . .
N201 N 0.0862(8) 0.3524(6) 0.3898(4) 0.090(4) Uiso 1 1 d D . .
N205 N 0.1882(7) 0.1075(5) 1.0482(3) 0.083(3) Uiso 1 1 d D . .
N209 N 0.6411(5) 0.0106(7) 1.1491(4) 0.101(4) Uiso 1 1 d D . .
N213 N 0.3956(5) 0.4923(5) 0.8765(3) 0.087(4) Uiso 1 1 d D . .
N217 N 0.953(1) 0.0761(7) 0.7821(4) 0.138(6) Uiso 1 1 d D . .
C5 C 1.0509(9) 0.1358(7) 0.3061(5) 0.073(4) Uiso 1 1 d . . .
C6 C 1.129(1) 0.1155(7) 0.2821(5) 0.078(4) Uiso 1 1 d . . .
C8 C 1.214(1) 0.1446(8) 0.2179(6) 0.094(5) Uiso 1 1 d . . .
C9 C 1.179(1) 0.108(1) 0.1816(7) 0.116(6) Uiso 1 1 d . . .
C11 C 1.034(1) 0.0840(9) 0.1290(6) 0.099(5) Uiso 1 1 d . . .
C12 C 0.970(1) 0.0580(7) 0.1554(5) 0.081(4) Uiso 1 1 d . . .
C14 C 0.872(1) 0.0786(7) 0.2182(5) 0.077(4) Uiso 1 1 d . . .
C15 C 0.930(1) 0.0782(7) 0.2652(5) 0.082(4) Uiso 1 1 d . . .
C17 C 0.7768(9) 0.0562(7) 0.4922(5) 0.072(4) Uiso 1 1 d . . .
C18 C 0.7617(9) 0.0117(7) 0.5294(5) 0.072(4) Uiso 1 1 d . . .
C20 C 0.734(1) 0.0103(9) 0.6118(6) 0.098(5) Uiso 1 1 d . . .
C21 C 0.720(1) 0.0619(8) 0.6512(6) 0.095(5) Uiso 1 1 d . . .

C23 C 0.8716(9) 0.1133(7) 0.6711(5) 0.074(4) Uiso 1 1 d . . .
C24 C 0.931(1) 0.0862(8) 0.6377(5) 0.085(4) Uiso 1 1 d . . .
C26 C 0.957(1) 0.0813(7) 0.5551(5) 0.076(4) Uiso 1 1 d . . .
C27 C 0.9243(9) 0.1130(7) 0.5111(5) 0.072(4) Uiso 1 1 d . . .
C29 C 0.6265(8) 0.0767(6) 0.8859(4) 0.060(3) Uiso 1 1 d . . .
C30 C 0.6142(8) 0.0346(6) 0.9252(4) 0.065(3) Uiso 1 1 d . . .
C32 C 0.6176(9) 0.0262(7) 1.0082(5) 0.075(4) Uiso 1 1 d . . .
C33 C 0.709(1) 0.0147(7) 1.0243(5) 0.079(4) Uiso 1 1 d . . .
C35 C 0.862(1) 0.0746(8) 1.0354(5) 0.084(4) Uiso 1 1 d . . .
C36 C 0.8873(9) 0.0681(7) 0.9873(5) 0.072(4) Uiso 1 1 d . . .
C38 C 0.8727(9) 0.1141(6) 0.9133(5) 0.069(3) Uiso 1 1 d . . .
C39 C 0.7870(8) 0.0820(6) 0.8865(4) 0.060(3) Uiso 1 1 d . . .
C40 C 0.9198(8) 0.1901(6) 0.2937(5) 0.064(3) Uani 1 1 d . . .
C41 C 0.8916(8) 0.1811(6) 0.3402(4) 0.060(3) Uani 1 1 d . . .
C42 C 0.9407(7) 0.2081(5) 0.3801(5) 0.056(3) Uani 1 1 d . . .
C43 C 0.9155(7) 0.2056(5) 0.4220(4) 0.054(3) Uani 1 1 d . . .
C44 C 0.8387(8) 0.1709(6) 0.4310(4) 0.060(3) Uani 1 1 d . . .
C45 C 0.7881(6) 0.1407(6) 0.3923(5) 0.058(3) Uani 1 1 d . . .
C46 C 0.8116(8) 0.1443(6) 0.3501(5) 0.062(3) Uani 1 1 d . . .
C47 C 0.8074(7) 0.1687(6) 0.4781(4) 0.059(3) Uani 1 1 d . . .
C48 C 0.7432(7) 0.1709(6) 0.6758(4) 0.056(3) Uani 1 1 d . . .
C49 C 0.7362(7) 0.1695(6) 0.7250(4) 0.059(3) Uani 1 1 d . . .
C50 C 0.8061(8) 0.1926(6) 0.7576(4) 0.055(3) Uani 1 1 d . . .
C51 C 0.7970(8) 0.1926(6) 0.8026(4) 0.058(3) Uani 1 1 d . . .
C52 C 0.7187(7) 0.1712(6) 0.8217(4) 0.057(3) Uani 1 1 d . . .
C53 C 0.6495(8) 0.1518(7) 0.7894(5) 0.068(4) Uani 1 1 d . . .
C54 C 0.6565(9) 0.1483(7) 0.7456(6) 0.077(4) Uani 1 1 d . . .
C55 C 0.7108(8) 0.1743(6) 0.8719(5) 0.063(3) Uani 1 1 d . . .
C56 C 0.9153(8) 0.2763(7) 0.1777(5) 0.065(3) Uani 1 1 d . . .
C58 C 0.8087(9) 0.3368(8) 0.1546(4) 0.072(4) Uani 1 1 d . . .
C60 C 0.7803(8) 0.2302(7) 0.1500(4) 0.064(3) Uani 1 1 d . . .
C69 C 0.958(1) 0.4262(7) 0.2785(5) 0.083(4) Uiso 1 1 d . . .
C70 C 1.032(1) 0.4596(8) 0.2537(6) 0.089(4) Uiso 1 1 d . . .
C72 C 1.064(1) 0.490(1) 0.1748(7) 0.112(6) Uiso 1 1 d . . .
C73 C 1.027(2) 0.559(1) 0.1735(8) 0.134(7) Uiso 1 1 d . . .
C75 C 0.884(1) 0.6045(9) 0.1629(6) 0.103(5) Uiso 1 1 d . . .
C76 C 0.858(1) 0.607(1) 0.2074(7) 0.113(6) Uiso 1 1 d . . .
C78 C 0.786(1) 0.5414(9) 0.2624(6) 0.103(5) Uiso 1 1 d . . .
C79 C 0.861(1) 0.5130(7) 0.2883(5) 0.083(4) Uiso 1 1 d . . .
C81 C 0.894(1) 0.4208(7) 0.4982(5) 0.083(4) Uiso 1 1 d . . .
C82 C 0.9390(9) 0.4489(6) 0.5414(5) 0.068(3) Uiso 1 1 d . . .
C84 C 0.915(1) 0.4551(7) 0.6251(5) 0.082(4) Uiso 1 1 d . . .
C85 C 0.847(1) 0.4313(9) 0.6591(6) 0.101(5) Uiso 1 1 d . . .
C87 C 0.714(1) 0.4868(7) 0.6438(5) 0.081(4) Uiso 1 1 d . . .
C88 C 0.742(1) 0.5333(8) 0.6079(6) 0.095(5) Uiso 1 1 d . . .
C90 C 0.773(1) 0.5315(8) 0.5273(5) 0.086(4) Uiso 1 1 d . . .
C91 C 0.7732(9) 0.4874(7) 0.4861(5) 0.070(3) Uiso 1 1 d . . .
C93 C 0.664(1) 0.5026(9) 0.8556(6) 0.101(5) Uiso 1 1 d . . .
C94 C 0.672(1) 0.553(1) 0.8867(7) 0.111(6) Uiso 1 1 d . . .
C96 C 0.632(1) 0.5829(8) 0.9701(6) 0.094(5) Uiso 1 1 d . . .

C97 C 0.693(2) 0.566(1) 0.9993(7) 0.122(6) Uiso 1 1 d . . .
C99 C 0.749(2) 0.466(1) 1.0282(8) 0.132(7) Uiso 1 1 d . . .
C100 C 0.802(2) 0.448(1) 0.9996(8) 0.133(7) Uiso 1 1 d . . .
C102 C 0.784(1) 0.3823(9) 0.9188(6) 0.101(5) Uiso 1 1 d . . .
C103 C 0.764(2) 0.421(2) 0.886(1) 0.18(1) Uiso 1 1 d . . .
C104 C 0.6315(8) 0.3827(6) 0.8481(4) 0.062(3) Uani 1 1 d . . .
C105 C 0.6539(9) 0.3774(7) 0.8012(5) 0.073(4) Uani 1 1 d . . .
C106 C 0.5982(8) 0.4067(8) 0.7680(5) 0.075(4) Uani 1 1 d . . .
C107 C 0.616(1) 0.4051(8) 0.7220(6) 0.090(5) Uani 1 1 d . . .
C108 C 0.6911(9) 0.3763(6) 0.7088(5) 0.070(4) Uani 1 1 d . . .
C109 C 0.740(1) 0.3500(7) 0.7392(5) 0.077(4) Uani 1 1 d . . .
C110 C 0.722(1) 0.3488(7) 0.7841(6) 0.088(5) Uani 1 1 d . . .
C111 C 0.7031(9) 0.3742(7) 0.6576(4) 0.072(4) Uani 1 1 d . . .
C112 C 0.7504(9) 0.3748(7) 0.4643(5) 0.081(4) Uani 1 1 d . . .
C113 C 0.7640(9) 0.3821(7) 0.4147(5) 0.075(4) Uani 1 1 d . . .
C114 C 0.7098(9) 0.4140(8) 0.3864(5) 0.078(4) Uani 1 1 d . . .
C115 C 0.7210(9) 0.4198(6) 0.3423(5) 0.071(4) Uani 1 1 d . . .
C116 C 0.7885(8) 0.3933(7) 0.3211(5) 0.070(4) Uani 1 1 d . . .
C117 C 0.8359(9) 0.3525(8) 0.3477(5) 0.083(4) Uani 1 1 d . . .
C118 C 0.8271(9) 0.3507(7) 0.3929(5) 0.073(4) Uani 1 1 d . . .
C119 C 0.8008(9) 0.4014(6) 0.2718(4) 0.063(3) Uani 1 1 d . . .
C120 C 0.7614(7) 0.2628(5) 0.5710(4) 0.051(3) Uani 1 1 d . . .
C122 C 0.6324(7) 0.1998(5) 0.5539(4) 0.044(2) Uani 1 1 d . . .
C124 C 0.6348(7) 0.3070(5) 0.5509(3) 0.050(3) Uani 1 1 d . . .
C133 C 0.553(1) 0.3098(8) 0.2097(5) 0.085(4) Uiso 1 1 d . . .
C134 C 0.516(1) 0.3278(9) 0.1627(6) 0.107(5) Uiso 1 1 d . . .
C136 C 0.5341(9) 0.3054(7) 0.0784(5) 0.075(4) Uiso 1 1 d . . .
C137 C 0.469(1) 0.254(1) 0.0685(7) 0.117(6) Uiso 1 1 d . . .
C139 C 0.4415(5) 0.1388(7) 0.0743(4) 0.074(4) Uiso 1 1 d D . .
C140 C 0.4073(6) 0.1301(9) 0.1203(3) 0.104(5) Uiso 1 1 d D . .
C142 C 0.470(1) 0.1418(8) 0.2048(5) 0.084(4) Uiso 1 1 d . . .
C143 C 0.470(1) 0.2045(9) 0.2163(6) 0.102(5) Uiso 1 1 d . . .
C145 C 0.404(1) 0.1725(7) 0.4336(5) 0.079(4) Uiso 1 1 d . . .
C146 C 0.3321(8) 0.1502(6) 0.4631(4) 0.062(3) Uiso 1 1 d . . .
C148 C 0.3026(9) 0.1400(7) 0.5458(5) 0.072(4) Uiso 1 1 d . . .
C149 C 0.354(1) 0.1591(7) 0.5937(5) 0.077(4) Uiso 1 1 d . . .
C151 C 0.357(1) 0.2744(7) 0.5989(5) 0.084(4) Uiso 1 1 d . . .
C152 C 0.3189(9) 0.2953(7) 0.5507(5) 0.073(4) Uiso 1 1 d . . .
C154 C 0.3558(9) 0.3069(6) 0.4714(5) 0.070(3) Uiso 1 1 d . . .
C155 C 0.424(1) 0.2875(7) 0.4395(5) 0.078(4) Uiso 1 1 d . . .
C157 C 0.2579(8) 0.1433(6) 0.8068(4) 0.063(3) Uiso 1 1 d . . .
C158 C 0.1783(8) 0.1262(6) 0.8294(4) 0.060(3) Uiso 1 1 d . . .
C160 C 0.1279(8) 0.1060(6) 0.9069(4) 0.059(3) Uiso 1 1 d . . .
C161 C 0.1088(8) 0.1672(6) 0.9275(4) 0.065(3) Uiso 1 1 d . . .
C163 C 0.1851(9) 0.2670(6) 0.9609(4) 0.067(3) Uiso 1 1 d . . .
C164 C 0.2052(9) 0.3018(6) 0.9207(5) 0.069(3) Uiso 1 1 d . . .
C166 C 0.3110(9) 0.3041(6) 0.8602(4) 0.067(3) Uiso 1 1 d . . .
C167 C 0.2776(8) 0.2587(6) 0.8228(4) 0.059(3) Uiso 1 1 d . . .
C168 C 0.6222(8) 0.2179(8) 0.2447(5) 0.083(5) Uani 1 1 d . . .
C169 C 0.5995(8) 0.2162(8) 0.2952(5) 0.068(4) Uani 1 1 d . . .

C170 C 0.597(1) 0.2751(9) 0.3189(5) 0.091(5) Uani 1 1 d . . .
C171 C 0.5797(9) 0.279(1) 0.3662(5) 0.102(6) Uani 1 1 d . . .
C172 C 0.5612(8) 0.2231(9) 0.3877(5) 0.079(4) Uani 1 1 d . . .
C173 C 0.5669(8) 0.1666(7) 0.3630(5) 0.069(4) Uani 1 1 d . . .
C174 C 0.5818(9) 0.1666(8) 0.3171(5) 0.073(4) Uani 1 1 d . . .
C175 C 0.5517(7) 0.2261(7) 0.4381(4) 0.066(3) Uani 1 1 d . . .
C176 C 0.4764(7) 0.2220(7) 0.6309(4) 0.068(4) Uani 1 1 d . . .
C177 C 0.4539(7) 0.2157(8) 0.6798(5) 0.067(4) Uani 1 1 d . . .
C178 C 0.4584(8) 0.2670(8) 0.7095(5) 0.076(4) Uani 1 1 d . . .
C179 C 0.4425(8) 0.2616(7) 0.7551(5) 0.071(4) Uani 1 1 d . . .
C180 C 0.4244(7) 0.2058(6) 0.7725(4) 0.058(3) Uani 1 1 d . . .
C181 C 0.4197(8) 0.1530(7) 0.7431(4) 0.063(3) Uani 1 1 d . . .
C182 C 0.4361(7) 0.1567(7) 0.6956(5) 0.065(3) Uani 1 1 d . . .
C183 C 0.4059(7) 0.1988(6) 0.8216(4) 0.057(3) Uani 1 1 d . . .
C184 C 0.6259(7) 0.2479(6) 0.9734(4) 0.049(3) Uani 1 1 d . . .
C186 C 0.5257(7) 0.3129(7) 0.9499(4) 0.061(3) Uani 1 1 d . . .
C188 C 0.4861(7) 0.2097(6) 0.9494(4) 0.056(3) Uani 1 1 d . . .
H5 H 0.9499 0.2304 0.2933 0.073 Uiso 1 1 calc . . .
H6 H 0.8681 0.1881 0.2730 0.073 Uiso 1 1 calc . . .
H7 H 0.9975 0.2294 0.3773 0.071 Uiso 1 1 calc . . .
H8 H 0.9500 0.2284 0.4460 0.064 Uiso 1 1 calc . . .
H9 H 0.7341 0.1173 0.3982 0.071 Uiso 1 1 calc . . .
H10 H 0.7770 0.1203 0.3253 0.076 Uiso 1 1 calc . . .
H11 H 0.7460 0.1652 0.4746 0.070 Uiso 1 1 calc . . .
H12 H 0.8293 0.2068 0.4938 0.070 Uiso 1 1 calc . . .
H13 H 0.7787 0.2088 0.6713 0.062 Uiso 1 1 calc . . .
H14 H 0.6863 0.1736 0.6622 0.062 Uiso 1 1 calc . . .
H15 H 0.8590 0.2094 0.7469 0.068 Uiso 1 1 calc . . .
H16 H 0.8445 0.2093 0.8236 0.070 Uiso 1 1 calc . . .
H17 H 0.5948 0.1417 0.7995 0.088 Uiso 1 1 calc . . .
H18 H 0.6081 0.1312 0.7250 0.089 Uiso 1 1 calc . . .
H19 H 0.6572 0.1909 0.8777 0.078 Uiso 1 1 calc . . .
H20 H 0.7577 0.2025 0.8863 0.078 Uiso 1 1 calc . . .
H21 H 0.6363 0.3427 0.8614 0.074 Uiso 1 1 calc . . .
H22 H 0.5717 0.3915 0.8484 0.074 Uiso 1 1 calc . . .
H23 H 0.5533 0.4283 0.7786 0.096 Uiso 1 1 calc . . .
H24 H 0.5771 0.4227 0.6996 0.103 Uiso 1 1 calc . . .
H25 H 0.7930 0.3336 0.7305 0.091 Uiso 1 1 calc . . .
H26 H 0.7556 0.3256 0.8048 0.107 Uiso 1 1 calc . . .
H27 H 0.6479 0.3729 0.6415 0.092 Uiso 1 1 calc . . .
H28 H 0.7294 0.3368 0.6504 0.092 Uiso 1 1 calc . . .
H29 H 0.7626 0.3344 0.4721 0.105 Uiso 1 1 calc . . .
H30 H 0.6873 0.3771 0.4666 0.105 Uiso 1 1 calc . . .
H31 H 0.6642 0.4326 0.3985 0.091 Uiso 1 1 calc . . .
H32 H 0.6826 0.4412 0.3246 0.079 Uiso 1 1 calc . . .
H33 H 0.8746 0.3280 0.3329 0.097 Uiso 1 1 calc . . .
H34 H 0.8651 0.3273 0.4115 0.089 Uiso 1 1 calc . . .
H35 H 0.7475 0.4122 0.2576 0.074 Uiso 1 1 calc . . .
H36 H 0.8141 0.3624 0.2590 0.074 Uiso 1 1 calc . . .
H37 H 0.6381 0.1770 0.2372 0.104 Uiso 1 1 calc . . .

H38 H 0.6723 0.2474 0.2442 0.104 Uiso 1 1 calc . . .
H39 H 0.6082 0.3112 0.3039 0.112 Uiso 1 1 calc . . .
H40 H 0.5826 0.3177 0.3827 0.117 Uiso 1 1 calc . . .
H41 H 0.5621 0.1284 0.3778 0.082 Uiso 1 1 calc . . .
H42 H 0.5802 0.1275 0.3001 0.086 Uiso 1 1 calc . . .
H43 H 0.5871 0.2625 0.4513 0.081 Uiso 1 1 calc . . .
H44 H 0.5755 0.1898 0.4500 0.081 Uiso 1 1 calc . . .
H45 H 0.5084 0.1882 0.6237 0.081 Uiso 1 1 calc . . .
H46 H 0.5116 0.2606 0.6301 0.081 Uiso 1 1 calc . . .
H47 H 0.4760 0.3080 0.6991 0.090 Uiso 1 1 calc . . .
H48 H 0.4440 0.2988 0.7748 0.081 Uiso 1 1 calc . . .
H49 H 0.4047 0.1131 0.7544 0.076 Uiso 1 1 calc . . .
H50 H 0.4341 0.1208 0.6764 0.084 Uiso 1 1 calc . . .
H51 H 0.4393 0.2320 0.8391 0.070 Uiso 1 1 calc . . .
H52 H 0.4258 0.1598 0.8300 0.070 Uiso 1 1 calc . . .
H53 H 1.1679 0.1988 0.2628 0.111 Uiso 1 1 calc . . .
H58 H 1.1178 0.1645 0.1364 0.115 Uiso 1 1 calc . . .
H63 H 0.8917 0.1236 0.1637 0.086 Uiso 1 1 calc . . .
H72 H 0.6715 0.0503 0.5603 0.082 Uiso 1 1 calc . . .
H73 H 0.9599 0.1552 0.5990 0.078 Uiso 1 1 calc . . .
H86 H 0.8975 0.1570 0.9727 0.080 Uiso 1 1 calc . . .
H91 H 0.5680 0.0897 0.9658 0.070 Uiso 1 1 calc . . .
H92 H 0.7462 0.0968 1.0588 0.080 Uiso 1 1 calc . . .
H101 H 1.0117 0.4103 0.1954 0.097 Uiso 1 1 calc . . .
H108 H 0.9312 0.5299 0.1180 0.149 Uiso 1 1 calc . . .
H109 H 0.7506 0.5449 0.1977 0.099 Uiso 1 1 calc . . .
H120 H 0.9127 0.3794 0.5847 0.084 Uiso 1 1 calc . . .
H121 H 0.6685 0.4981 0.5555 0.084 Uiso 1 1 calc . . .
H138 H 0.5613 0.5352 0.9084 0.105 Uiso 1 1 calc . . .
H139 H 0.6244 0.4989 1.0271 0.099 Uiso 1 1 calc . . .
H152 H 0.7285 0.3679 0.9820 0.111 Uiso 1 1 calc . . .
H157 H 0.6279 0.3239 0.1382 0.128 Uiso 1 1 calc . . .
H158 H 0.5407 0.1902 0.0503 0.126 Uiso 1 1 calc . . .
H159 H 0.5118 0.0942 0.1471 0.107 Uiso 1 1 calc . . .
H176 H 0.3994 0.1101 0.5124 0.078 Uiso 1 1 calc . . .
H177 H 0.4227 0.3382 0.5294 0.072 Uiso 1 1 calc . . .
H210 H 0.2295 0.0756 0.8776 0.064 Uiso 1 1 calc . . .
H211 H 0.2008 0.1767 0.9794 0.073 Uiso 1 1 calc . . .
H212 H 0.3350 0.3033 0.9266 0.067 Uiso 1 1 calc . . .

loop_
_atom_site_aniso_label
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_atom_site_aniso_U_33
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_atom_site_aniso_U_13
_atom_site_aniso_U_23
 Zn1 0.0581(9) 0.115(1) 0.072(1) 0.0178(9) 0.0136(8) 0.008(1)
 Zn2 0.0384(7) 0.0653(9) 0.0672(9) 0.0110(6) 0.0039(6) 0.0067(7)

Zn3 0.0388(7) 0.071(1) 0.076(1) 0.0069(7) 0.0030(6) 0.0168(8)
Zn65 0.0521(9) 0.082(1) 0.087(1) -0.0105(8) -0.0021(8) 0.0209(9)
Zn66 0.0472(8) 0.0654(9) 0.076(1) -0.0179(7) 0.0198(7) -0.0060(7)
Zn67 0.0378(7) 0.0692(9) 0.0641(9) -0.0085(6) 0.0118(6) 0.0011(7)
Zn129 0.0434(7) 0.077(1) 0.0604(9) 0.0058(7) 0.0147(6) 0.0075(7)
Zn130 0.0358(7) 0.073(1) 0.0603(9) 0.0001(6) 0.0042(6) -0.0001(7)
Zn131 0.0310(6) 0.0595(8) 0.0645(8) 0.0022(6) 0.0061(6) 0.0070(7)
S62 0.048(2) 0.104(3) 0.110(3) -0.007(2) 0.004(2) 0.025(2)
S63 0.085(3) 0.076(2) 0.083(3) 0.000(2) -0.012(2) 0.009(2)
S64 0.047(2) 0.068(2) 0.086(2) 0.004(2) 0.012(2) 0.006(2)
S126 0.037(1) 0.071(2) 0.083(2) 0.002(1) -0.003(1) -0.003(2)
S127 0.045(2) 0.048(2) 0.102(3) -0.001(1) -0.002(2) 0.002(2)
S128 0.042(2) 0.055(2) 0.083(2) 0.006(1) 0.004(1) 0.001(2)
S190 0.042(2) 0.073(2) 0.088(2) -0.001(1) -0.009(2) 0.000(2)
S191 0.038(1) 0.057(2) 0.071(2) 0.001(1) 0.013(1) 0.004(1)
S192 0.038(1) 0.062(2) 0.072(2) -0.002(1) 0.000(1) 0.010(2)
N57 0.073(8) 0.09(1) 0.082(8) -0.014(7) 0.015(6) 0.012(7)
N59 0.048(6) 0.063(7) 0.066(7) -0.003(5) 0.004(5) 0.001(5)
N61 0.040(5) 0.101(9) 0.064(6) 0.019(6) 0.014(5) 0.020(6)
N121 0.035(5) 0.052(6) 0.050(5) 0.003(4) 0.004(4) -0.007(4)
N123 0.045(5) 0.051(6) 0.056(6) -0.007(5) 0.012(4) -0.007(4)
N125 0.033(5) 0.050(6) 0.061(6) -0.009(4) 0.003(4) -0.002(4)
N185 0.023(4) 0.065(7) 0.070(6) -0.011(4) 0.008(4) 0.011(5)
N187 0.031(4) 0.054(6) 0.070(6) -0.010(4) 0.010(4) -0.004(5)
N189 0.032(5) 0.053(6) 0.072(6) -0.011(4) 0.008(4) -0.006(5)
C40 0.057(7) 0.055(7) 0.077(9) -0.002(6) 0.006(6) -0.017(6)
C41 0.052(7) 0.062(8) 0.067(8) 0.003(6) 0.015(6) 0.014(6)
C42 0.041(6) 0.050(7) 0.074(9) -0.008(5) 0.005(6) -0.001(6)
C43 0.036(6) 0.053(7) 0.070(8) -0.002(5) -0.007(6) -0.002(6)
C44 0.057(7) 0.062(8) 0.063(8) 0.025(6) -0.002(6) -0.001(6)
C45 0.025(5) 0.066(8) 0.083(9) 0.000(5) 0.009(6) 0.009(7)
C46 0.047(7) 0.056(7) 0.082(9) 0.008(6) -0.003(6) 0.009(7)
C47 0.039(6) 0.070(8) 0.071(8) 0.010(6) 0.015(6) 0.009(6)
C48 0.039(6) 0.065(8) 0.065(8) 0.013(5) 0.008(5) 0.011(6)
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