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#
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*******
data MACUKI
database code depnum ccdc archive 'CCDC 1533360'
audit update record
2017-02-17 deposited with the CCDC.
2019-01-11 downloaded from the CCDC.
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space group symop operation xyz
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 [Sheldrick, G.M. (2014). SADABS Bruker AXS Inc., Madison, Wisconsin,
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# DATA COLLECTION # # --\_\_\_\_\_ ---# \_diffrn\_measurement\_method 'rotation images' diffrn\_detector '(CMOS) PHOTON 100' \_diffrn\_ambient\_temperature 150(2) \_diffrn\_radiation\_wavelength 0.71073 \_diffrn\_radiation\_type MoK∖a \_diffrn\_radiation\_probe \_diffrn\_radiation\_probe x-ray \_diffrn\_radiation\_source 'Incoatec microfocus sealed tube' diffrn radiation monochromator 'multilayer monochromator' diffrn reflns av r equivalents 0.0969 \_diffrn\_reflns\_av\_uneti/neti 0.0948 21560 -11 diffrn reflns number diffrn reflns limit h min \_diffrn\_reflns\_limit\_h\_max 11 \_diffrn\_reflns\_limit\_k\_min -14 14 -18 18 \_diffrn\_reflns\_limit\_k\_max \_diffrn\_reflns\_limit\_l\_min \_diffrn\_reflns\_limit\_l max \_diffrn\_reflns theta min 2.913 \_diffrn\_reflns theta max 27.484 diffrn measured fraction theta full 0.997 \_diffrn\_measured\_fraction theta max 0.998 \_reflns\_number\_total 6186 \_reflns\_number gt 4930 \_reflns\_threshold expression >2sigma(I) #\_\_\_\_\_\_ ---# # COMPUTER PROGRAMS USED # ---# \_computing\_data\_collection 'SAINT (Bruker, 2014)'
\_computing\_cell\_refinement 'APEX3 (Bruker, 2015); SAINT (Bruker, 2014)' \_computing\_data\_reduction 'SAINT (Bruker, 2014)' \_computing\_structure\_solution 'SHELXT (Sheldrick, 2015)' \_computing\_structure\_refinement 'SHELXL-2016/6 (Sheldrick, 2016)' 2014)' computing publication material 'CRYSCALC (T. Roisnel, local program, 2016)' #--------# # REFINEMENT INFORMATION # #\_\_\_\_\_ ---# 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  $F^{2^{-1}}$ . 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. \_refine\_ls\_structure\_factor coef Fsqd refine ls matrix type full \_refine\_ls\_weighting scheme calc refine ls weighting details  $w=1/[s^{2}(Fo^{2})+(0.0864P)^{2}]$  where  $P=(Fo^{2}+2Fc^{2})/3$ ? atom sites solution primary \_atom\_sites\_solution\_secondary ? \_atom\_sites\_solution\_hydrogens geom \_refine\_ls\_hydrogen\_treatment constr \_refine\_ls\_extinction method none \_refine\_ls\_extinction\_coef \_refine\_ls number reflns 6186 refine ls number parameters 261 refine ls number restraints 0 \_refine\_ls\_R\_factor all 0.0762 \_refine\_ls\_R\_factor gt 0.0584 refine ls wR factor ref 0.1622 \_refine\_ls\_wR\_factor gt 0.1497 \_refine\_ls\_goodness of fit ref 1.057 refine ls restrained S all 1.057 refine ls shift/su max 0.024 refine ls shift/su mean 0.002 \_refine\_diff\_density\_max 2.688 \_refine\_diff\_density\_min -2.488 \_refine\_diff\_density\_rms 0.278 \_shelx\_res\_file ; .res SHELXL file: MACuKI.res #------TITL import a.res in P-1 MACuKI.res created by SHELXL-2016/6 at 15:06:07 on 10-Feb-2017 CELL 0.71073 8.8160 10.9385 14.2052 91.625 97.465 95.545 ZERR 0.0008 0.0009 0.0013 0.003 0.003 0.003 2.00 LATT 1 SFAC C Н CU 0 S I K Ρ 2 UNIT 40 40 2 10 2 4 4 MERG 2 EADP C7 C8 C9 C10 C11 C12 FMAP 2 20 PLAN 0.25 0.33 0.60 SIZE ACTA BOND \$H CONF

LIST 4 WPDB -2 L.S. 4 TEMP -123.00 WGHT 0.086400 FVAR 0.26772 CU1 3 0.832085 0.791599 0.320877 11.00000 0.01461 0.01674 =0.01505 0.00061 0.00029 0.00182 II 6 0.967151 0.688531 0.468041 11.00000 0.01344 0.02348 =0.01933 0.00728 -0.00088 0.00255 6 0.964451 1.008844 0.304821 11.00000 0.02252 I2 0.01624 =0.02457 0.00514 0.00410 0.00076 P1 8 0.698174 0.684549 0.197476 11.00000 0.01103 0.01825 = 0.01248 0.00096 0.00013 0.00331 7 0.674348 0.426302 0.452328 11.00000 К1 0.01609 0.02461 =0.03691 0.01310 0.00405 0.00682 7 0.262472 0.964270 0.505073 11.00000 0.01906 K2 0.02021 =0.02184 -0.00103 0.00314 0.00230 s1 5 0.485645 0.733210 0.372323 11.00000 0.01181 0.01508 =0.01466 0.00182 0.00259 0.00308 01 4 0.614563 0.828585 0.386643 11.00000 0.01586 0.01998 =0.01775 -0.00091 0.00099 0.00110 02 4 0.531762 0.610768 0.386850 11.00000 0.02686 0.01430 =0.02217 0.00643 0.00138 0.00591 03 0.364358 0.760971 0.428250 11.00000 4 0.01739 0.02698 = 0.02421 -0.00072 0.00856 0.00701 4 0.353582 0.335873 0.406116 11.00000 04 0.02467 0.03453 =0.02534 0.00362 -0.00030 0.00007 4 0.532202 0.901930 0.611280 11.00000 0.04147 05 0.03689 =0.02950 0.00023 0.00087 0.01331 c1 1 0.761330 0.717934 0.082846 11.00000 0.00969 0.02446 =0.01350 0.00566 -0.00130 0.00425 C2 1 0.780032 0.842125 0.058573 11.00000 0.01953 0.03170 =0.01708 0.00564 -0.00079 0.00388 AFIX 43 0.754069 0.904207 0.100016 11.00000 -1.20000 Н2 2 AFIX 0 1 0.874717 -0.025206 11.00000 0.835959 C3 0.02391 0.04256 =0.02168 0.01545 -0.01023 -0.01427 AFIX 43 2 H.3 0.843913 0.958160 -0.042413 11.00000 -1.20000 AFIX 0

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C15 1 0.566109 0.312128 0.162807 11.00000 0.02135 0.02031 = 0.03155 0.00218 0.00017 -0.00477 AFIX 43 2 H15 0.479086 0.259009 0.135231 11.00000 -1.20000 AFIX O C16 1 0.694218 0.263664 0.205848 11.00000 0.02692 0.02107 =0.03234 -0.00011 0.00274 0.00432 AFIX 43 2 0.695615 0.177025 0.207653 11.00000 -1.20000 H16 AFIX 0 C17 1 0.822410 0.340896 0.246964 11.00000 0.02214 0.02814 =0.02278 0.00462 0.00030 0.00571 AFIX 43 H17 2 0.910147 0.306853 0.277475 11.00000 -1.20000 AFIX 0 1 0.821575 0.466621 0.243253 11.00000 C18 0.01005 0.02783 =0.01877 -0.00286 -0.00146 0.00234 AFIX 43 H18 2 0.909651 0.519112 0.270099 11.00000 -1.20000 AFIX 0 c19 1 0.261575 0.371414 0.323167 11.00000 0.02247 0.05321 =0.02304 0.00569 -0.00151 0.00418 AFIX 137 H19A20.2024290.4381960.34019811.00000-1.50000H19B20.1908770.3008900.29597411.00000-1.50000H19C20.3282280.3995660.27635911.00000-1.50000 AFIX 0 C20 1 0.581116 0.944519 0.707772 11.00000 0.03480 0.03025 =0.04535 0.00701 0.00453 0.00694 AFIX 137 0.5061400.9963130.72872411.00000-1.500000.6817690.9924890.71216411.00000-1.500000.5888940.8738820.74842211.00000-1.50000 H20A 2 H20B 2 H20C 2 AFIX 0 hklf 4

REM import\_a.res in P-1 REM R1 = 0.0584 for 4930 Fo > 4sig(Fo) and 0.0762 for all 6186 data REM 261 parameters refined using 0 restraints END WGHT 0.0885 0.0000 REM Highest difference peak 2.688, deepest hole -2.488, 1-sigma level 0.278 Q1 1 0.8868 0.6434 0.4397 11.00000 0.05 2.69

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Q2

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Q.6
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Q9
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011
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Q12

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      0.05

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Q16
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Q17
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Q18 1 0.2878 0.2959 0.4512 11.00000 0.05
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atom site fract x \_atom\_site\_fract V \_atom\_site\_fract z \_atom\_site\_U\_iso\_or\_equiv atom site adp type atom site occupancy atom site site symmetry order atom site calc flag atom site refinement flags posn \_atom\_site\_refinement\_flags\_adp \_atom\_site\_refinement\_flags occupancy \_atom\_site\_disorder assembly \_atom\_site\_disorder\_group Cul Cu 0.83208(9) 0.79160(6) 0.32088(5) 0.01560(19) Uani 1 1 d . . . . I1 I 0.96715(5) 0.68853(4) 0.46804(3) 0.01885(14) Uani 1 1 d . . . . I2 I 0.96445(5) 1.00884(3) 0.30482(3) 0.02102(14) Uani 1 1 d . . . . P1 P 0.69817(18) 0.68455(14) 0.19748(11) 0.0139(3) Uani 1 1 d . . . K1 K 0.67435(17) 0.42630(13) 0.45233(11) 0.0253(3) Uani 1 1 d . . . K2 K 0.26247(16) 0.96427(12) 0.50507(10) 0.0203(3) Uani 1 1 d . . S1 S 0.48564(17) 0.73321(13) 0.37232(10) 0.0136(3) Uani 1 1 d . . . . 01 0 0.6146(5) 0.8286(4) 0.3866(3) 0.0181(9) Uani 1 1 d . . . . 02 0 0.5318(5) 0.6108(4) 0.3869(3) 0.0209(10) Uani 1 1 d . . . . O3 O 0.3644(5) 0.7610(4) 0.4282(3) 0.0221(10) Uani 1 1 d . . . . 04 0 0.3536(6) 0.3359(5) 0.4061(3) 0.0287(11) Uani 1 1 d . . . . O5 O 0.5322(7) 0.9019(5) 0.6113(4) 0.0357(13) Uani 1 1 d . . . C1 C 0.7613(7) 0.7179(6) 0.0828(4) 0.0159(12) Uani 1 1 d . . . C2 C 0.7800(8) 0.8421(6) 0.0586(5) 0.0229(14) Uani 1 1 d . . H2 H 0.754069 0.904207 0.100016 0.027 Uiso 1 1 calc R U . . . C3 C 0.8360(8) 0.8747(7) -0.0252(5) 0.0314(17) Uani 1 1 d . . . H3 H 0.843913 0.958160 -0.042413 0.038 Uiso 1 1 calc R U . . . C4 C 0.8801(9) 0.7846(8) -0.0835(5) 0.0343(18) Uani 1 1 d . . . H4 H 0.921170 0.806706 -0.139969 0.041 Uiso 1 1 calc R U . . . C5 C 0.8646(9) 0.6626(8) -0.0600(5) 0.0326(17) Uani 1 1 d . . . H5 H 0.896336 0.601675 -0.100095 0.039 Uiso 1 1 calc R U . . . C6 C 0.8033(8) 0.6282(7) 0.0215(4) 0.0250(15) Uani 1 1 d . . . H6 H 0.789777 0.543843 0.035844 0.030 Uiso 1 1 calc R U . . . C7 C 0.4928(8) 0.7125(6) 0.1761(5) 0.0226(6) Uani 1 1 d . . . C8 C 0.4197(8) 0.7132(6) 0.0838(5) 0.0226(6) Uani 1 1 d . . . H8 H 0.475891 0.699737 0.032448 0.027 Uiso 1 1 calc R U . . . C9 C 0.2656(7) 0.7332(6) 0.0650(5) 0.0226(6) Uani 1 1 d . . . . H9 H 0.217918 0.732266 0.000998 0.027 Uiso 1 1 calc R U . . . C10 C 0.1815(8) 0.7542(6) 0.1375(5) 0.0226(6) Uani 1 1 d . . . H10 H 0.076706 0.769410 0.124321 0.027 Uiso 1 1 calc R U . . . C11 C 0.2526(8) 0.7528(6) 0.2307(5) 0.0226(6) Uani 1 1 d . . H11 H 0.194794 0.764829 0.281568 0.027 Uiso 1 1 calc R U . . C12 C 0.4070(8) 0.7340(6) 0.2507(5) 0.0226(6) Uani 1 1 d . . . C13 C 0.6906(7) 0.5175(5) 0.1998(4) 0.0149(12) Uani 1 1 d . . . . C14 C 0.5636(8) 0.4389(6) 0.1595(5) 0.0203(13) Uani 1 1 d . . . . H14 H 0.474698 0.472086 0.129646 0.024 Uiso 1 1 calc R U . . . C15 C 0.5661(8) 0.3121(6) 0.1628(5) 0.0251(15) Uani 1 1 d . . . . H15 H 0.479086 0.259009 0.135231 0.030 Uiso 1 1 calc R U . . . C16 C 0.6942(8) 0.2637(6) 0.2058(5) 0.0268(15) Uani 1 1 d . . . H16 H 0.695615 0.177025 0.207653 0.032 Uiso 1 1 calc R U . . . C17 C 0.8224(8) 0.3409(6) 0.2470(5) 0.0243(14) Uani 1 1 d . . . H17 H 0.910147 0.306853 0.277475 0.029 Uiso 1 1 calc R U . . . C18 C 0.8216(7) 0.4666(6) 0.2433(4) 0.0192(13) Uani 1 1 d . . . H18 H 0.909651 0.519112 0.270099 0.023 Uiso 1 1 calc R U . . . C19 C 0.2616(9) 0.3714(8) 0.3232(5) 0.0332(17) Uani 1 1 d . . . .

H19A H 0.202429 0.438196 0.340198 0.050 Uiso 1 1 calc R U . . . H19B H 0.190877 0.300890 0.295974 0.050 Uiso 1 1 calc R U . . H19C H 0.328228 0.399566 0.276359 0.050 Uiso 1 1 calc R U . . . C20 C 0.5811(10) 0.9445(7) 0.7078(6) 0.0365(18) Uani 1 1 d . . . . H20A H 0.506140 0.996313 0.728724 0.055 Uiso 1 1 calc R U . . . H20B H 0.681769 0.992489 0.712164 0.055 Uiso 1 1 calc R U . . . H2OC H 0.588894 0.873882 0.748422 0.055 Uiso 1 1 calc R U . . . loop atom site aniso label \_atom\_site\_aniso\_U\_11 \_atom\_site\_aniso\_U\_ 22 \_atom\_site\_aniso\_U\_33 \_atom\_site\_aniso U 23 \_atom\_site\_aniso U 13 atom site aniso U 12 Cul 0.0146(4) 0.0167(4) 0.0151(4) 0.0006(3) 0.0003(3) 0.0018(3) I1 0.0134(2) 0.0235(2) 0.0193(2) 0.00728(16) -0.00088(16) 0.00255(16) I2 0.0225(3) 0.0162(2) 0.0246(2) 0.00514(17) 0.00410(18) 0.00076(17) P1 0.0110(7) 0.0182(7) 0.0125(7) 0.0010(6) 0.0001(6) 0.0033(6) K1 0.0161(7) 0.0246(7) 0.0369(9) 0.0131(6) 0.0041(6) 0.0068(6) K2 0.0191(7) 0.0202(6) 0.0218(7) -0.0010(5) 0.0031(6) 0.0023(5) S1 0.0118(7) 0.0151(7) 0.0147(7) 0.0018(5) 0.0026(6) 0.0031(5) 01 0.016(2) 0.020(2) 0.018(2) -0.0009(18) 0.0010(18) 0.0011(18) 02 0.027(3) 0.014(2) 0.022(2) 0.0064(18) 0.001(2) 0.0059(19) 03 0.017(2) 0.027(2) 0.024(2) -0.0007(19) 0.009(2) 0.0070(19) 04 0.025(3) 0.035(3) 0.025(3) 0.004(2) 0.000(2) 0.000(2) 05 0.041(3) 0.037(3) 0.030(3) 0.000(2) 0.001(2) 0.013(3) C1 0.010(3) 0.024(3) 0.014(3) 0.006(2) -0.001(2) 0.004(2) C2 0.020(3) 0.032(4) 0.017(3) 0.006(3) -0.001(3) 0.004(3) C3 0.024(4) 0.043(4) 0.022(3) 0.015(3) -0.010(3) -0.014(3) C4 0.031(4) 0.054(5) 0.014(3) 0.007(3) -0.001(3) -0.012(4) C5 0.026(4) 0.055(5) 0.016(3) -0.007(3) 0.004(3) 0.004(4)C6 0.031(4) 0.033(4) 0.011(3) 0.001(3) 0.003(3) 0.004(3) C7 0.0150(14) 0.0308(14) 0.0218(14) -0.0006(12) -0.0009(11) 0.0061(11) C8 0.0150(14) 0.0308(14) 0.0218(14) -0.0006(12) -0.0009(11) 0.0061(11) C9 0.0150(14) 0.0308(14) 0.0218(14) -0.0006(12) -0.0009(11) 0.0061(11) C10 0.0150(14) 0.0308(14) 0.0218(14) -0.0006(12) -0.0009(11) 0.0061(11) C11 0.0150(14) 0.0308(14) 0.0218(14) -0.0006(12) -0.0009(11) 0.0061(11) C12 0.0150(14) 0.0308(14) 0.0218(14) -0.0006(12) -0.0009(11) 0.0061(11) C13 0.018(3) 0.016(3) 0.012(3) 0.002(2) 0.005(2) 0.006(2) C14 0.017(3) 0.021(3) 0.022(3) 0.001(3) 0.003(3) 0.001(3) C15 0.021(4) 0.020(3) 0.032(4) 0.002(3) 0.000(3) -0.005(3) C16 0.027(4) 0.021(3) 0.032(4) 0.000(3) 0.003(3) 0.004(3) C17 0.022(4) 0.028(3) 0.023(3) 0.005(3) 0.000(3) 0.006(3) C18 0.010(3) 0.028(3) 0.019(3) -0.003(3) -0.001(2) 0.002(3) C19 0.022(4) 0.053(5) 0.023(4) 0.006(3) -0.002(3) 0.004(3) C20 0.035(5) 0.030(4) 0.045(5) 0.007(3) 0.005(4) 0.007(3) ---# # MOLECULAR GEOMETRY # #\_\_\_\_\_\_ ---#

\_geom\_special\_details

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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.
;
loop
geom bond atom site label 1
geom bond atom site label 2
geom bond distance
_geom_bond_site_symmetry 2
geom bond publ flag
Cul P1 2.2173(17) . ?
Cul Ol 2.304(4) . ?
Cul I2 2.5739(8) . ?
Cul Il 2.6087(9) . ?
Cul K2 3.8119(15) 2 676 ?
I1 K1 3.5729(15) 2 766 ?
I1 K1 3.6502(16) . ?
I1 K2 3.7668(14) 1 655 ?
I2 K2 3.5852(14) 2 676 ?
I2 K2 3.6901(16) 1 655 ?
P1 C1 1.823(6) . ?
P1 C13 1.823(6) . ?
P1 C7 1.853(7) . ?
K1 O2 2.610(5) . ?
K1 03 2.721(5) 2 666 ?
K1 04 2.889(5) . ?
K1 O2 3.110(5) 2 666 ?
K1 O4 3.290(5) 2 666 ?
K1 C18 3.415(7) . ?
K1 S1 3.453(2) 2_666 ?
K1 C17 3.487(7) . ?
K1 K1 3.975(3) 2 666 ?
K1 K2 4.410(2) 2 666 ?
K2 O3 2.729(4) . ?
K2 01 2.751(4) 2 676 ?
K2 O5 2.799(6) . ?
K2 O5 2.925(6) 2 676 ?
K2 K2 4.207(3) 2 676 ?
K2 K2 4.752(3) 2_576 ?
S1 O2 1.449(4) . ?
S1 O1 1.456(4) . ?
S1 O3 1.462(4) . ?
S1 C12 1.777(7) . ?
O4 C19 1.427(9) . ?
O5 C20 1.433(9) . ?
C1 C6 1.402(9) . ?
C1 C2 1.411(9) . ?
C2 C3 1.389(9) . ?
C2 H2 0.9500 . ?
C3 C4 1.386(12) . ?
C3 H3 0.9500 . ?
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C4 C5 1.383(11) . ? C4 H4 0.9500 . ? C5 C6 1.387(10) . ? C5 H5 0.9500 . ? С6 Н6 0.9500 . ? C7 C8 1.384(9) . ? C7 C12 1.405(9) . ? C8 C9 1.389(9) . ? C8 H8 0.9500 . ? C9 C10 1.372(9) . ? С9 Н9 0.9500 . ? C10 C11 1.391(9) . ? C10 H10 0.9500 . ? C11 C12 1.390(9) . ? C11 H11 0.9500 . ? C13 C14 1.393(9) . ? C13 C18 1.408(9) . ? C14 C15 1.391(9) . ? C14 H14 0.9500 . ? C15 C16 1.373(10) . ? C15 H15 0.9500 . ? C16 C17 1.396(10) . ? C16 H16 0.9500 . ? C17 C18 1.378(9) . ? C17 H17 0.9500 . ? C18 H18 0.9500 . ? C19 H19A 0.9800 . ? С19 Н19В 0.9800 . ? C19 H19C 0.9800 . ? C20 H20A 0.9800 . ? C20 H20B 0.9800 . ? C20 H20C 0.9800 . ? loop\_ \_geom\_angle\_atom\_site\_label 1 \_geom\_angle\_atom\_site\_label\_2 \_geom\_angle\_atom\_site\_label\_3 \_geom\_angle \_geom\_angle\_site\_symmetry\_1 \_geom\_angle\_site\_symmetry 3 geom angle publ flag P1 Cu1 01 92.92(11) . . ? P1 Cu1 I2 121.90(5) . . ? 01 Cul I2 103.19(11) . . ? P1 Cu1 I1 122.86(5) . . ? O1 Cu1 I1 96.30(11) . . ? I2 Cul I1 110.42(3) . . ? P1 Cu1 K2 133.92(5) . 2 676 ? O1 Cu1 K2 45.69(10) . 2 676 ? I2 Cu1 K2 64.97(3) . 2 676 ? I1 Cu1 K2 86.93(3) . 2<sup>-</sup>676 ? Cul I1 K1 139.72(3) . 2 766 ? Cul I1 K1 93.86(3) . . ? K1 I1 K1 106.44(3) 2\_766 . ? Cul Il K2 88.75(3) . 1 655 ? K1 I1 K2 73.81(3) 2 766 1 655 ? K1 I1 K2 175.22(3) . 1 655 ? Cu1 I2 K2 74.45(3) . 2 676 ?

Cu1 I2 K2 90.98(3) . 1 655 ? K2 I2 K2 81.55(4) 2\_676 1\_655 ? C1 P1 C13 103.2(3) . . ? C1 P1 C7 101.9(3) . . ? C13 P1 C7 103.3(3) . . ? C1 P1 Cu1 115.1(2) . . ? C13 P1 Cu1 117.2(2) . . ? C7 P1 Cu1 114.2(2) . . ? O2 K1 O3 139.26(15) . 2\_666 ? 02 K1 04 73.33(15) . . ? O3 K1 O4 76.10(15) 2\_666 . ? O2 K1 O2 92.41(13) . 2\_666 ? O3 K1 O2 48.50(12) 2 666 2 666 ? O4 K1 O2 59.97(13) . 2 666 ? O2 K1 O4 59.91(13) . 2 666 ? O3 K1 O4 100.70(13) 2\_666 2\_666 ? O4 K1 O4 100.22(12) . 2\_666 ? 02 K1 04 61.80(12) 2\_666 2\_666 ? O2 K1 C18 79.17(15) . . ? O3 K1 C18 136.36(15) 2\_666 . ? O4 K1 C18 107.51(15) . . ? O2 K1 C18 166.82(15) 2 666 . ? O4 K1 C18 120.48(15) 2 666 . ? O2 K1 S1 116.03(11) . 2 666 ? O3 K1 S1 23.82(9) 2\_666 2\_666 ? O4 K1 S1 64.46(11) . 2 666 ? O2 K1 S1 24.82(8) 2 666 2 666 ? O4 K1 S1 82.44(10) 2\_666 2\_666 ? C18 K1 S1 157.08(12) . 2 666 ? 02 K1 C17 98.58(16) . . ? O3 K1 C17 113.58(15) 2\_666 . ? O4 K1 C17 101.70(16) . . ? O2 K1 C17 154.89(15) 2 666 . ? . ? O4 K1 C17 142.76(15) 2\_666 C18 K1 C17 23.01(15) . . ? S1 K1 C17 134.38(12) 2 666 . ? O2 K1 I1 147.46(12) . 2\_766 ? O3 K1 I1 69.04(10) 2\_666 2\_766 ? O4 K1 I1 138.96(11) . 2\_766 ? 02 K1 I1 107.40(9) 2 666 2 766 ? 04 K1 I1 106.79(10) 2 666 2 766 ? C18 K1 I1 84.73(11) . 2 766 ? S1 K1 I1 88.88(4) 2 666 2 766 ? C17 K1 I1 74.28(12) . 2\_766 ? O2 K1 I1 74.21(11) . . ? O3 K1 I1 130.55(11) 2\_666 . ? O4 K1 I1 147.47(11) . . ? O2 K1 I1 119.76(9) 2 666 . ? O4 K1 I1 60.87(9) 2 666 . ? C18 K1 I1 67.95(11) . . ? S1 K1 I1 130.89(5) 2\_666 . ? C17 K1 I1 85.07(12) . . ? I1 K1 I1 73.56(3) 2\_766 . ? O2 K1 K1 51.43(10) . 2\_666 ? O3 K1 K1 88.80(10) 2 666 2 666 ? O4 K1 K1 54.56(10) . 2 666 ? O2 K1 K1 40.99(8) 2 666 2 666 ? O4 K1 K1 45.67(9) 2 666 2 666 ?

C18 K1 K1 129.68(12) . 2 666 ? S1 K1 K1 65.03(5) 2 666 2 666 ? C17 K1 K1 143.75(13) . 2\_666 ? I1 K1 K1 141.94(7) 2\_766 2\_666 ? I1 K1 K1 102.11(5) . 2 666 ? O2 K1 K2 155.75(11) . 2 666 ? O3 K1 K2 36.04(9) 2 666 2 666 ? O4 K1 K2 83.93(11) . 2 666 ? O2 K1 K2 83.15(8) 2\_666 2\_666 ? 04 K1 K2 134.68(10) 2\_666 2\_666 ? C18 K1 K2 100.33(11) . 2 666 ? S1 K1 K2 58.53(4) 2\_666 2\_666 ? C17 K1 K2 77.56(12) . 2 666 ? I1 K1 K2 55.11(3) 2\_766<sup>2</sup>\_666 ? I1 K1 K2 128.46(4) . 2 666 ? K1 K1 K2 120.35(6) 2\_666 2\_666 ? O3 K2 O1 137.85(14) . 2\_676 ? O3 K2 O5 68.40(14) . . ? O1 K2 O5 73.79(14) 2\_676 . ? O3 K2 O5 84.05(14) . 2\_676 ? O1 K2 O5 74.87(14) 2\_676 2\_676 ? O5 K2 O5 85.40(17) . 2 676 ? O3 K2 I2 129.88(11) . 2 676 ? O1 K2 I2 72.95(9) 2\_676 2\_676 ? O5 K2 I2 98.51(12) . 2 676 ? O5 K2 I2 144.97(10) 2 676 2 676 ? O3 K2 I2 96.57(11) . 1 455 ? 01 K2 I2 116.36(10) 2\_676 1\_455 ? O5 K2 I2 162.28(11) . 1\_455 ? O5 K2 I2 83.66(11) 2 676 1 455 ? I2 K2 I2 98.45(4) 2 676 1 455 ? O3 K2 I1 65.82(10) . 1 455 ? O1 K2 I1 148.33(10) 2\_676 1\_455 ? O5 K2 I1 110.05(12) . 1 455 ? O5 K2 I1 135.94(11) 2 676 1 455 ? I2 K2 I1 75.40(3) 2\_676 1\_455 ? I2 K2 I1 69.60(3) 1\_455 1\_455 ? O3 K2 Cu1 163.33(11) . 2\_676 ? O1 K2 Cu1 36.82(9) 2\_676 2\_676 ? O5 K2 Cu1 97.59(11) . 2 676 ? O5 K2 Cu1 104.41(10) 2 676 2 676 ? I2 K2 Cu1 40.578(19) 2 676 2 676 ? I2 K2 Cu1 98.61(4) 1 455 2 676 ? I1 K2 Cu1 113.50(4) 1 455 2 676 ? O3 K2 K2 71.52(10) . 2 676 ? O1 K2 K2 68.46(10) 2\_676 2\_676 ? O5 K2 K2 43.86(12) . 2 676 ? O5 K2 K2 41.54(11) 2 676 2 676 ? I2 K2 K2 131.89(5) 2 676 2 676 ? I2 K2 K2 123.85(5) 1 455 2 676 ? I1 K2 K2 136.69(5) 1 455 2 676 ? Cu1 K2 K2 105.12(5) 2 676 2 676 ? O3 K2 K1 35.92(10) . 2\_666 ? O1 K2 K1 130.43(11) 2\_676 2\_666 ? O5 K2 K1 60.56(11) . 2\_666 ? 05 K2 K1 116.85(11) 2 676 2 666 ? I2 K2 K1 94.70(4) 2 676 2 666 ? I2 K2 K1 112.85(4) 1 455 2 666 ?

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I1 K2 K1 51.08(3) 1 455 2 666 ?
Cu1 K2 K1 129.64(4) 2 676 2 666 ?
K2 K2 K1 89.25(5) 2_676 2_666 ?
O3 K2 K2 124.93(11) . 2_576 ?
O1 K2 K2 97.10(10) 2 676 2 576 ?
O5 K2 K2 148.36(13) . 2 576 ?
O5 K2 K2 122.14(12) 2 676 2 576 ?
I2 K2 K2 50.18(3) 2 676 2 576 ?
I2 K2 K2 48.27(3) 1_455 2 576 ?
I1 K2 K2 62.56(3) 1 455 2 576 ?
Cu1 K2 K2 62.82(3) 2_676 2_576 ?
K2 K2 K2 159.43(7) 2_676 2_576 ?
K1 K2 K2 111.30(5) 2 666 2 576 ?
O2 S1 O1 113.1(3) . . ?
O2 S1 O3 112.6(3) . . ?
O1 S1 O3 111.4(3) . . ?
O2 S1 C12 105.7(3) . . ?
O1 S1 C12 106.5(3) . . ?
O3 S1 C12 107.1(3) . . ?
O2 S1 K1 64.25(19) . 2_666 ?
O1 S1 K1 126.31(18) . 2 666 ?
O3 S1 K1 48.75(19) . 2 666 ?
C12 S1 K1 126.3(2) . 2 666 ?
S1 O1 Cu1 117.2(2) . . ?
S1 O1 K2 143.9(2) . 2_676 ?
Cul Ol K2 97.49(15) . 2 676 ?
S1 O2 K1 162.7(3) . . ?
S1 O2 K1 90.9(2) . 2_666 ?
K1 O2 K1 87.59(13) . 2_666 ?
S1 O3 K1 107.4(2) . 2_666 ?
S1 O3 K2 137.6(3) . . ?
K1 O3 K2 108.04(15) 2_666 . ?
C19 O4 K1 122.0(4) . . ?
C19 O4 K1 98.7(4) . 2 666 ?
K1 O4 K1 79.78(12) . 2 666 ?
C20 O5 K2 123.2(4) . . ?
C20 O5 K2 106.8(4) . 2_676 ?
K2 O5 K2 94.60(16) . 2_676 ?
C6 C1 C2 118.6(6) . . ?
C6 C1 P1 123.5(5) . . ?
C2 C1 P1 117.7(5) . . ?
C3 C2 C1 120.8(6) . . ?
C3 C2 H2 119.6 . . ?
C1 C2 H2 119.6 . . ?
C4 C3 C2 119.5(7) . .
                      ?
C4 C3 H3 120.3 . . ?
C2 C3 H3 120.3 . . ?
C5 C4 C3 120.4(7) . . ?
C5 C4 H4 119.8 . . ?
C3 C4 H4 119.8 . . ?
C4 C5 C6 120.7(7) . . ?
C4 C5 H5 119.6 . . ?
C6 C5 H5 119.6 . . ?
C5 C6 C1 120.0(7) . . ?
С5 С6 Н6 120.0 . . ?
C1 C6 H6 120.0 . . ?
C8 C7 C12 118.1(6) . . ?
C8 C7 P1 119.5(5) . . ?
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C12 C7 P1 122.4(5) . . ? C7 C8 C9 121.2(6) . . ? С7 С8 Н8 119.4 . . ? C9 C8 H8 119.4 . . ? C10 C9 C8 120.9(6) . . ? С10 С9 Н9 119.6 . . ? С8 С9 Н9 119.6 . . ? C9 C10 C11 118.7(6) . . ? C9 C10 H10 120.7 . . ? C11 C10 H10 120.7 . . ? C10 C11 C12 121.1(6) . . C10 C11 H11 119.5 . . ? C12 C11 H11 119.5 . . ? C11 C12 C7 120.0(6) . . ? C11 C12 S1 117.2(5) . . ? C7 C12 S1 122.7(5) . . ? C14 C13 C18 119.0(6) . . ? C14 C13 P1 123.3(5) . . ? C18 C13 P1 117.7(5) . . ? C15 C14 C13 120.3(6) . . ? C15 C14 H14 119.8 . . ? C13 C14 H14 119.8 . . ? C16 C15 C14 120.1(6) . . ? C16 C15 H15 120.0 . . ? C14 C15 H15 120.0 . . ? C15 C16 C17 120.4(6) . . ? C15 C16 H16 119.8 . . ? C17 C16 H16 119.8 . . ? C18 C17 C16 119.9(6) . . C18 C17 K1 75.6(4) . . ? C16 C17 K1 97.2(4) . . ? C18 C17 H17 120.0 . . ? C16 C17 H17 120.0 . . ? К1 С17 Н17 97.1 . . ? C17 C18 C13 120.2(6) . . ? C17 C18 K1 81.4(4) . . ? C13 C18 K1 93.2(4) . . ? C17 C18 H18 119.9 . . ? C13 C18 H18 119.9 . . ? K1 C18 H18 95.3 . . ? 04 C19 H19A 109.5 . . ? O4 C19 H19B 109.5 . . ? H19A C19 H19B 109.5 . . ? O4 C19 H19C 109.5 . . ? H19A C19 H19C 109.5 . . ? H19B C19 H19C 109.5 . . ? O5 C20 H20A 109.5 . . ? O5 C20 H20B 109.5 . . ? H20A C20 H20B 109.5 . . ? O5 C20 H20C 109.5 . . ? H20A C20 H20C 109.5 . . ? H20B C20 H20C 109.5 . . ?

loop\_

\_geom\_torsion\_atom\_site\_label\_1 \_geom\_torsion\_atom\_site\_label\_2 \_geom\_torsion\_atom\_site\_label\_3 \_geom\_torsion\_atom\_site\_label\_4

\_geom\_torsion \_geom\_torsion\_site\_symmetry 1 \_geom\_torsion\_site\_symmetry\_2 \_geom\_torsion\_site\_symmetry\_3 geom torsion site symmetry 4 geom torsion publ flag 02 S1 O1 Cu1 44.3(3) . . . ? 03 S1 O1 Cu1 172.2(3) . . . ? C12 S1 O1 Cu1 -71.4(3) . . . ? K1 S1 O1 Cu1 118.40(19) 2\_666 . . . ? 02 S1 O1 K2 -118.4(4) . . . 2\_676 ? O3 S1 O1 K2 9.5(5) . . . 2\_676 ? C12 S1 O1 K2 126.0(4) . . . 2 676 ? K1 S1 O1 K2 -44.3(5) 2\_666 . . 2\_676 ? 01 S1 O2 K1 35.7(10) . . . ? O3 S1 O2 K1 -91.6(10) . . . ? C12 S1 O2 K1 151.9(9) . . . ? K1 S1 O2 K1 -84.9(9) 2 666 . . . ? 01 S1 O2 K1 120.6(2) . . . 2\_666 ? O3 S1 O2 K1 -6.7(3) . . . 2\_666 ? C12 S1 O2 K1 -123.2(2) . . . 2\_666 ? O2 S1 O3 K1 8.1(3) . . . 2 666 ? O1 S1 O3 K1 -120.1(2) . . . 2 666 ? C12 S1 O3 K1 123.7(3) . . . 2 666 ? O2 S1 O3 K2 153.6(3) . . . ? O1 S1 O3 K2 25.4(5) . . . ? C12 S1 O3 K2 -90.7(4) . . . ? K1 S1 O3 K2 145.5(5) 2 666 . . . ? C13 P1 C1 C6 -4.8(6) . . . ? C7 P1 C1 C6 -111.7(6) . . . ? Cul P1 C1 C6 124.1(5) . . . ? C13 P1 C1 C2 -179.7(5) . . . ? C7 P1 C1 C2 73.4(5) . . . ? Cu1 P1 C1 C2 -50.8(5) . . . . ? C6 C1 C2 C3 1.3(10) . . . ? P1 C1 C2 C3 176.4(5) . . . ? C1 C2 C3 C4 -2.8(10) . . . ? C2 C3 C4 C5 1.8(11) . . . ? C3 C4 C5 C6 0.7(11) . . . ? C4 C5 C6 C1 -2.3(11) . . . ? C2 C1 C6 C5 1.3(10) . . . ? P1 C1 C6 C5 -173.6(6) . . . C1 P1 C7 C8 19.0(6) . . . ? C13 P1 C7 C8 -87.8(6) . . . ? Cul P1 C7 C8 143.8(5) . . . . C1 P1 C7 C12 -160.6(6) . . . ? C13 P1 C7 C12 92.5(6) . . . ? Cu1 P1 C7 C12 -35.8(7) . . . ? C12 C7 C8 C9 -0.7(10) . . . ? P1 C7 C8 C9 179.7(5) . . . ? C7 C8 C9 C10 0.7(11) . . . ? C8 C9 C10 C11 -1.2(11) . . . ? C9 C10 C11 C12 1.8(10) . . . ? C10 C11 C12 C7 -1.8(11) . . . ? C10 C11 C12 S1 -179.7(5) . . . ? C8 C7 C12 C11 1.2(10) . . . ? P1 C7 C12 C11 -179.1(5) . . . ? C8 C7 C12 S1 179.0(5) . . .

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P1 C7 C12 S1 -1.4(9) . . . ?
O2 S1 C12 C11 117.0(6) . . . ?
O1 S1 C12 C11 -122.5(6) . . . ?
O3 S1 C12 C11 -3.2(6) . . . ?
K1 S1 C12 C11 47.7(7) 2 666 . . . ?
O2 S1 C12 C7 -60.8(7) . . . ?
O1 S1 C12 C7 59.7(6) . . . ?
O3 S1 C12 C7 179.0(6) . . . ?
K1 S1 C12 C7 -130.1(5) 2 666 . . . ?
C1 P1 C13 C14 -85.3(6) . . . ?
C7 P1 C13 C14 20.6(6) . . . ?
Cul P1 C13 C14 147.1(5) . . . ?
C1 P1 C13 C18 93.5(5) . . . ?
C7 P1 C13 C18 -160.6(5) . . . ?
Cul P1 C13 C18 -34.1(5) . . . ?
C18 C13 C14 C15 0.4(9) . . . ?
P1 C13 C14 C15 179.2(5) . . . ?
C13 C14 C15 C16 0.0(10) . . . ?
C14 C15 C16 C17 0.3(11) . . . ?
C15 C16 C17 C18 -0.9(11) . . . ?
C15 C16 C17 K1 76.5(7) . . . ?
C16 C17 C18 C13 1.3(10) . . . ?
K1 C17 C18 C13 -88.8(6) . . . ?
C16 C17 C18 K1 90.0(6) . . . ?
C14 C13 C18 C17 -1.0(9) . . . ?
P1 C13 C18 C17 -179.9(5) . . . ?
C14 C13 C18 K1 -83.0(5) . . . ?
P1 C13 C18 K1 98.1(4) . . .
                         ?
#______
---#
#===END OF CIF FILE FOR MACUKI
#
#_____
---#
*****
# This file contains crystal structure data downloaded from the
# Cambridge Structural Database (CSD) hosted by the Cambridge
# Crystallographic Data Centre (CCDC).
#
# Full information about CCDC data access policies and citation
# guidelines are available at http://www.ccdc.cam.ac.uk/access/V1
#
# Audit and citation data items may have been added by the CCDC.
# Please retain this information to preserve the provenance of
# this file and to allow appropriate attribution of the data.
*****
data MACUKI2
database code depnum ccdc archive 'CCDC 1533368'
_audit_update_record
2017-02-17 deposited with the CCDC.
2019-01-11 downloaded from the CCDC.
;
```

\_\_\_\_\_ ---# # CHEMICAL INFORMATION # #\_\_\_\_\_\_ ---# chemical name systematic ; ? ; \_chemical\_formula\_moiety 'C36 H28 Cu K O6 P2 S2' \_chemical\_formula\_sum \_chemical\_formula\_weight 'C36 H28 Cu K O6 P2 S2' 785.28 \_chemical\_compound\_source 'synthesis as described' #\_\_\_\_\_ ---# # UNIT CELL INFORMATION # #--------# \_space\_group\_crystal\_system triclinic space\_group\_name H-M alt 'P -1' '-P 1' \_space\_group\_name\_Hall \_space\_group\_IT\_number 2 loop space group symop operation xyz 'x, y, z' '-x, -y, -z' \_cell\_length\_a 10.3800(4) \_cell\_length\_b 11.5408(4)\_cell\_length\_c 14.0557(4) \_cell\_angle\_alpha 87.0640(10) 86.3820(10) \_cell\_angle beta cell angle gamma 86.7850(10) 1675.86(10) cell volume \_cell\_formula\_units\_Z 2 \_cell\_measurement\_theta\_min2.38\_cell\_measurement\_theta\_max27.50\_cell\_measurement\_wavelength0.710 0.71073 ---# # CRYSTAL INFORMATION # ---# \_exptl\_crystal\_description prism exptl crystal colour colourless

0.160 \_exptl\_crystal\_size\_max \_exptl\_crystal\_size\_mid 0.100 0.080 \_exptl\_crystal\_size\_min \_exptl\_crystal\_density\_meas ? \_exptl\_crystal\_density\_diffrn 1.556 exptl crystal density method ? exptl crystal F 000 804 exptl special details ; ? ; #\_\_\_\_\_ ---# # ABSORPTION CORRECTION # #\_\_\_\_\_\_ ---# exptl absorpt coefficient mu 1.043 \_exptl\_absorpt\_correction\_type multi-scan exptl absorpt process details ; [Sheldrick, G.M. (2014). SADABS Bruker AXS Inc., Madison, Wisconsin, USA] exptl absorpt correction T min 0.811 exptl absorpt correction T max 0.920 #\_\_\_\_\_\_ ---# # DATA COLLECTION # \_\_\_# \_diffrn\_measurement\_device\_type \_diffrn\_measurement\_method 'D8 VENTURE Bruker AXS' \_diffrn\_detector '(CMOS) PHOTON 100' \_diffrn\_ambient\_temperature 150 \_diffrn\_radiation\_wavelength 0.71073 \_diffrn\_radiation\_type MoK\a diffrn radiation type MoK∖a \_diffrn\_radiation\_probe \_diffrn\_radiation\_probe x-ray \_diffrn\_radiation\_source 'Incoatec microfocus sealed tube' \_diffrn\_reflns\_av\_r\_equivalents 0.0255 \_diffrn\_reflns\_av\_uneti/neti 0.0321 19961 \_diffrn\_reflns number -13 diffrn reflns limit h min diffrn reflns limit h max 13 diffrn reflns limit k min -14 \_diffrn\_reflns\_limit\_k\_max 13 \_diffrn\_reflns\_limit\_l\_min -18 \_diffrn\_reflns\_limit\_l\_max 18 \_diffrn\_reflns\_theta\_min 3.057 \_diffrn\_reflns\_theta\_max 27.481 \_diffrn\_reflns\_theta\_full 25.242 diffrn measured fraction theta full 0.982

diffrn measured fraction theta max 0.983 \_reflns\_number total 7559 \_reflns\_number\_gt 6806 reflns threshold expression >2sigma(I) #\_\_\_\_\_ ---# # COMPUTER PROGRAMS USED # \_\_\_\_\_ # \_ \_ ---# \_computing\_data\_collection 'SAINT (Bruker, 2014)'
\_computing\_cell\_refinement 'APEX3 (Bruker, 2015); 'APEX3 (Bruker, 2015); SAINT (Bruker, 2014)' \_computing data reduction 'SAINT (Bruker, 2014)' computing structure solution 'SHELXT (Sheldrick, 2015)' \_computing\_structure\_refinement 'SHELXL-2016/6 (Sheldrick, 2016)' computing\_molecular\_graphics 'SXGRAPH (Farrugia, 1999), Mercury (CSD, 2016)' computing publication material 'CRYSCALC (T. Roisnel, local program, 2016)' #\_\_\_\_\_\_ ---# REFINEMENT INFORMATION # ---# \_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  $F^{2^{-1}}$ . 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  $F^{2^{-1}}$  are statistically about twice as large as those based on F, and Rfactors based on ALL data will be even larger. \_refine\_ls\_structure\_factor coef Fsqd \_refine\_ls\_matrix\_type full \_refine\_ls\_weighting\_scheme calc refine ls weighting details  $w=1/[s^2(Fo^2)+(0.0351P)^2+1.0890P]$  where  $P=(Fo^2+2Fc^2)/3$ \_atom\_sites\_solution primary ? atom sites solution secondary ? atom sites solution hydrogens geom constr \_refine\_ls\_extinction\_coef 7559 \_refine\_ls\_number reflns \_refine\_ls\_number\_parameters 433 refine ls number restraints 0 refine ls R factor all 0.0331

0.0280 \_refine\_ls\_R\_factor\_gt \_refine\_ls\_wR\_factor\_ref 0.0827 \_refine\_ls\_wR\_factor\_gt 0.0735 \_refine\_ls\_goodness\_of\_fit\_ref 1.134 \_refine\_ls\_restrained\_S\_all 1.134 refine ls shift/su max 0.020 \_refine\_ls shift/su mean 0.003 refine diff density max 0.661 \_refine\_diff\_density\_min -0.508 \_refine\_diff\_density rms 0.084 #..... . . . . . . . # .RES SHELXL file: job.res # .HKL SHELXL file: job.hkl . . . . . . . \_shelx\_res file ; TITL import a.res in P-1 job.res created by SHELXL-2016/6 at 11:30:33 on 15-Feb-2017 CELL 0.71073 10.3800 11.5408 14.0557 87.064 86.382 86.785 2.0 0.0004 0.0004 0.0004 0.001 0.001 ZERR 0.001 LATT 1 SFAC C Η CU 0 S K Ρ 2 4 56 UNIT 72 12 2 4 MERG 2 FMAP 2 PLAN 20 ACTA BOND \$H CONF LIST 4 WPDB -2 L.S. 4 TEMP -123.00 WGHT 0.035100 1.089000 FVAR 0.45278 CU1 3 0.324968 0.444878 0.222395 11.00000 0.01709 0.01060 = 0.01364 -0.00103 0.00038 -0.00031 7 0.349987 0.252983 0.247419 11.00000 0.01532 P1 0.01067 =0.01204 0.00015 -0.00090 -0.00008 0.520826 0.206762 0.248895 11.00000 C11 0.01772 0.01036 =0.02461 -0.00111 -0.00244 -0.00084 C2 0.597815 0.215512 0.163577 11.00000 1 0.02311 0.01712 =0.03146 0.00052 0.00361 -0.00023 AFIX 43 Н2 2 0.558964 0.235552 0.105146 11.00000 -1.20000 AFIX 0 1 C3 0.731117 0.194886 0.164321 11.00000 0.02219 0.01682 = 0.06060 -0.00348 0.01264 -0.00250

AFIX 43 0.782930 0.199390 0.106208 11.00000 -1.20000 2 HЗ AFIX O 1 0.788641 0.167725 0.249805 11.00000 0.01596 C4 0.01804 =0.08644 -0.00571 -0.00850 -0.00078 AFIX 43 H4 2 0.879731 0.154161 0.250196 11.00000 -1.20000 AFIX O C5 1 0.713406 0.160476 0.334071 11.00000 0.02833 0.02506 =0.06095 -0.00155 -0.02449 -0.00223 AFIX 43 0.753145 0.142621 0.392480 11.00000 -1.20000 Н5 2 AFIX 0 1 0.579570 0.179104 0.334341 11.00000 0.02567 C6 0.01973 = 0.03055 -0.00094 -0.01011 -0.00236 AFIX 43 0.528363 0.172980 0.392650 11.00000 -1.20000 2 Hб AFIX 0 1 0.274375 0.186008 0.355951 11.00000 C7 0.01787 0.01879 = 0.01438 0.00296 -0.00164 -0.00013 C8 1 0.239256 0.254306 0.431909 11.00000 0.04288 0.02132 =0.02411 0.00041 0.00877 0.00307 AFIX 43 0.254487 0.334849 0.426526 11.00000 -1.20000 Н8 2 AFIX 0 C9 1 0.181916 0.207504 0.516319 11.00000 0.04111 0.03980 =0.02180 0.00056 0.01112 0.01275 AFIX 43 0.161477 0.255348 0.568784 11.00000 -1.20000 Н9 2 AFIX 0 1 0.154864 0.092244 0.523833 11.00000 C10 0.03554 0.04373 =0.02290 0.01321 0.00699 -0.00172 AFIX 43 0.114695 0.060296 0.581115 11.00000 -1.20000 H10 2 AFIX 0 c11 1 0.185991 0.023791 0.448556 11.00000 0.09714 0.03326 =0.03152 0.00758 0.01324 -0.02608 AFIX 43 H11 2 0.166085 -0.055724 0.453222 11.00000 -1.20000 AFIX 0 C12 1 0.246814 0.069725 0.364828 11.00000 0.08569 0.02289 =0.02320 -0.00038 0.01357 -0.01606 AFIX 43 0.269570 0.020823 0.313382 11.00000 -1.20000 H12 2 AFIX 0 C13 1 0.290336 0.170350 0.152361 11.00000 0.01736 0.01324 =0.01323 -0.00070 0.00131 -0.00269

1 0.352178 0.064818 0.126699 11.00000 0.02429 C14 0.01509 = 0.02018 -0.00112 -0.00135 0.00194 AFIX 43 2 H14 0.427228 0.036722 0.157745 11.00000 -1.20000AFIX O 11.00000 0.03885 C15 1 0.305898 0.000149 0.056551 0.01456 =0.02538 -0.00751 -0.00093 0.00147 AFIX 43 -0.071720 0.040322 11.00000 -1.20000 H15 2 0.348683 AFIX 0 C16 1 0.196989 0.041142 0.010440 11.00000 0.04285 0.02139 =0.02264 -0.00776 -0.00786 -0.00415 AFIX 43 H16 2 0.165297 -0.002727 -0.037614 11.00000 -1.20000 AFIX 0 1 C17 0.133930 0.146183 0.034214 11.00000 0.02770 0.02133 =0.02067 -0.00199 -0.00619 -0.00320 AFIX 43 H17 2 0.059428 0.173983 0.002366 11.00000 -1.20000 AFIX 0 C18 1 0.179921 0.210373 0.104502 11.00000 0.01763 0.01374 =0.01370 0.00037 0.00151 -0.00138 s1 5 0.092560 0.343079 0.133686 11.00000 0.01202 0.01617 =0.01742 -0.00141 -0.00072 -0.00010 01 4 -0.012771 0.356971 0.070256 11.00000 0.01983 0.02869 =0.03998 -0.00523 -0.01420 0.00221 0.052521 0.328590 0.233738 11.00000 024 0.02484 0.02731 =0.02226 -0.00239 0.01101 -0.00277 03 4 0.184624 0.435595 0.115517 11.00000 0.01714 0.01476 =0.01716 0.00179 -0.00081 -0.00033 7 0.281153 0.603260 0.304208 11.00000 0.01340 P2 0.01254 =0.01290 -0.00232 0.00178 -0.00138 c21 1 0.243827 0.586970 0.433202 11.00000 0.02108 0.01843 =0.01472 -0.00308 0.00321 -0.00553 0.330617 0.520276 0.487741 11.00000 0.02739 C22 1 0.03517 =0.02009 -0.00122 0.00085 0.00303 AFIX 43 H22 2 0.405695 0.484069 0.457496 11.00000 -1.20000 AFIX 0 1 0.586457 11.00000 C23 0.308073 0.506272 0.03970 0.04498 = 0.02029 0.00460 -0.00525 -0.00174 AFIX 43 0.368419 0.461835 0.623384 11.00000 -1.20000 H23 2 AFIX 0

1 0.198120 0.557012 0.630288 11.00000 0.04179 C24 0.04101 = 0.01446 -0.00098 0.00495 -0.01408 AFIX 43 2 0.183017 H24 0.547857 0.697551 11.00000 -1.20000 AFIX O C25 1 0.109643 0.621228 0.576731 11.00000 0.03367 0.05030 =0.02089 - 0.00516 0.01066 - 0.00134AFIX 43 0.033036 0.654833 0.606923 11.00000 -1.20000 H25 2 AFIX 0 1 0.133323 0.636443 0.478279 11.00000 0.02845 C26 0.03575 =0.01930 -0.00246 0.00508 0.00323 AFIX 43 H26 2 0.072902 0.681293 0.441708 11.00000 -1.20000 AFIX 0 1 0.696007 0.262842 C27 0.145871 11.00000 0.01529 0.01625 =0.01457 -0.00103 0.00324 0.00112 C28 1 0.030340 0.644074 0.250316 11.00000 0.01960 0.02038 = 0.03422 -0.00597 -0.00115 -0.00110 AFIX 43 H28 2 0.025388 0.562332 0.259994 11.00000 -1.20000 0 AFIX C29 1 -0.077361 0.711869 0.223711 11.00000 0.01869 0.03634 =0.03832 -0.00647 -0.00479 -0.00001 AFIX 43 H29 2 -0.156580 0.676679 0.216719 11.00000 -1.20000 AFIX 0 1 -0.069586 0.830831 0.207319 11.00000 0.02216 C30 0.03810 = 0.02415 0.00671 0.00218 0.01090 AFIX 43 2 Н30 -0.143575 0.876916 0.189208 11.00000 -1.20000 AFIX 0 C31 1 0.044468 0.882247 0.217141 11.00000 0.03010 0.02282 =0.04896 0.01295 0.00384 0.00516 AFTX 43 H31 2 0.049730 0.963668 0.205219 11.00000 -1.20000 AFIX 0 C32 1 0.152694 0.814757 0.244665 11.00000 0.02064 0.01972 =0.04529 0.00473 0.00126 -0.00179 AFIX 43 0.231773 0.850464 0.251013 11.00000 -1.20000 НЗ2 2 AFIX 0 1 0.413305 0.703932 0.296919 11.00000 C33 0.01419 0.01660 =0.01726 -0.00267 -0.00152 -0.00082 C34 1 0.430312 0.773135 0.373385 11.00000 0.02562 0.02560 =0.02039 -0.00842 0.00325 -0.00703 AFIX 43

НЗ4 2 0.378561 0.762419 0.431025 11.00000 -1.20000 AFIX 0 1 0.521304 0.857191 0.366769 11.00000 C35 0.02850 0.03245 =0.03114 -0.01493 -0.00084 -0.01144 AFIX 43 Н35 2 0.903490 0.419548 11.00000 0.531128 -1.20000 AFIX 0 C36 1 0.597585 0.873706 0.283690 11.00000 0.02184 0.02579 =0.03975 -0.00996 0.00144 -0.01083 AFIX 43 0.932494 0.278793 НЗ6 2 0.658488 11.00000 -1.20000 AFIX 0 C37 1 0.585311 0.804560 0.207488 11.00000 0.01543 0.02026 =0.02768 -0.00212 0.00279 -0.00387 AFIX 43 Н37 2 0.638661 0.815467 0.150646 11.00000 -1.20000 AFIX 0 C38 1 0.495054 0.718960 0.213687 11.00000 0.01217 0.01410 =0.01700 -0.00216 -0.00027 0.00024 4 0.598873 0.664219 0.048728 11.00000 0.02526 021 0.02265 =0.02321 -0.00193 0.01308 -0.00565 022 4 0.363287 0.671753 0.071175 11.00000 0.02263 0.02876 =0.01960 -0.00365 -0.00587 0.00170 0.493740 0.512382 0.143024 11.00000 0.02036 023 4 0.01422 =0.02133 -0.00224 0.00744 -0.00137 S2 5 0.486645 0.635983 0.110157 11.00000 0.01463 0.01561 =0.01404 -0.00255 0.00322 -0.00148 6 0.248048 0.541774 -0.047509 11.00000 0.01928 K1 0.02184 =0.01731 0.00169 -0.00164 0.00058 4 HKLF

REM import a.res in P-1 REM R1 = 0.0280 for 6806 Fo > 4sig(Fo) and 0.0331 for all 7559 data REM 433 parameters refined using 0 restraints END WGHT 0.0429 0.9661 REM Highest difference peak 0.661, deepest hole -0.508, 1-sigma level 0.084 0.66 01 1 0.5001 0.5788 0.1414 11.00000 0.05 Q2 1 0.1349 0.2660 0.1193 11.00000 0.05 0.34 1 0.5714 0.8553 0.2389 11.00000 0.05 0.34 Q3 Q4 1 0.5475 0.2042 0.2879 11.00000 0.05 0.33

```
05
    1 0.5518 0.8660 0.3224 11.00000 0.05 0.33
     1 0.2427 -0.0801 0.4649 11.00000 0.05
                                                  0.32
Q6

      1
      0.12127
      0.00011
      0.1013
      11.00000
      0.032

      1
      0.1850
      0.1076
      0.0253
      11.00000
      0.05
      0.32

      1
      0.4163
      0.2347
      0.3391
      11.00000
      0.05
      0.32

      1
      0.0355
      0.3800
      0.0326
      11.00000
      0.05
      0.32

Q7
Q.8
Q.9
Q10 1 0.4469 0.7237 0.3449 11.00000 0.05 0.31
    1 0.4696 0.8232 0.3626 11.00000 0.05 0.31
Q11
    1 0.3368 0.0389 0.0825 11.00000 0.05 0.31
012
013 1 0.2549 0.0211 0.0400 11.00000 0.05 0.30
     1 0.3655 0.3664 0.2811 11.00000 0.05 0.29
Q14
     10.17340.18330.057511.000000.050.2910.20550.66020.273911.000000.050.29
015
Q16
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Q17
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Q18 1 0.2764 0.5196 0.1535 11.00000 0.05
                                                  0.28
Q19 1 0.2984 0.3763 0.2686 11.00000 0.05 0.28
Q20 1 -0.0454 0.7655 0.1968 11.00000 0.05 0.28
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# ..... End of .HKL file
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#
              ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS
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Cul Cu 0.32497(2) 0.44488(2) 0.22240(2) 0.01383(7) Uani 1 1 d . . . .
P1 P 0.34999(4) 0.25298(4) 0.24742(3) 0.01272(10) Uani 1 1 d . . . .
C1 C 0.52083(18) 0.20676(16) 0.24889(14) 0.0175(4) Uani 1 1 d . . . .
C2 C 0.5978(2) 0.21551(17) 0.16358(16) 0.0242(4) Uani 1 1 d . .
H2 H 0.558964 0.235552 0.105146 0.029 Uiso 1 1 calc R U . .
C3 C 0.7311(2) 0.19489(19) 0.1643(2) 0.0337(5) Uani 1 1 d . . .
H3 H 0.782930 0.199390 0.106208 0.040 Uiso 1 1 calc R U . . .
C4 C 0.7886(2) 0.1677(2) 0.2498(2) 0.0398(6) Uani 1 1 d . . .
H4 H 0.879731 0.154161 0.250196 0.048 Uiso 1 1 calc R U . . .
C5 C 0.7134(2) 0.1605(2) 0.3341(2) 0.0372(6) Uani 1 1 d . . . .
H5 H 0.753145 0.142621 0.392480 0.045 Uiso 1 1 calc R U . . .
C6 C 0.5796(2) 0.17910(18) 0.33434(16) 0.0249(4) Uani 1 1 d .
H6 H 0.528363 0.172980 0.392650 0.030 Uiso 1 1 calc R U .
                                                         .
C7 C 0.27438(18) 0.18601(17) 0.35595(13) 0.0171(4) Uani 1 1 d . . . .
C8 C 0.2393(2) 0.2543(2) 0.43191(16) 0.0301(5) Uani 1 1 d . . . .
H8 H 0.254487 0.334849 0.426526 0.036 Uiso 1 1 calc R U . . .
C9 C 0.1819(3) 0.2075(2) 0.51632(16) 0.0354(6) Uani 1 1 d . . . .
H9 H 0.161477 0.255348 0.568784 0.042 Uiso 1 1 calc R U . . .
C10 C 0.1549(2) 0.0922(2) 0.52383(16) 0.0350(5) Uani 1 1 d . . . .
H10 H 0.114695 0.060296 0.581115 0.042 Uiso 1 1 calc R U . . .
C11 C 0.1860(4) 0.0238(2) 0.44856(19) 0.0542(9) Uani 1 1 d . .
H11 H 0.166085 -0.055724 0.453222 0.065 Uiso 1 1 calc R U . . .
C12 C 0.2468(3) 0.0697(2) 0.36483(17) 0.0442(7) Uani 1 1 d . . . .
H12 H 0.269570 0.020823 0.313382 0.053 Uiso 1 1 calc R U . . .
C13 C 0.29034(18) 0.17035(16) 0.15236(12) 0.0146(3) Uani 1 1 d . . . .
C14 C 0.3522(2) 0.06482(17) 0.12670(14) 0.0200(4) Uani 1 1 d . . . .
H14 H 0.427228 0.036722 0.157745 0.024 Uiso 1 1 calc R U . . .
C15 C 0.3059(2) 0.00015(18) 0.05655(15) 0.0262(4) Uani 1 1 d . . . .
H15 H 0.348683 -0.071720 0.040322 0.031 Uiso 1 1 calc R U . . .
C16 C 0.1970(2) 0.04114(19) 0.01044(15) 0.0284(5) Uani 1 1 d . . . .
H16 H 0.165297 -0.002727 -0.037614 0.034 Uiso 1 1 calc R U . .
C17 C 0.1339(2) 0.14618(18) 0.03421(14) 0.0229(4) Uani 1 1 d . . . .
H17 H 0.059428 0.173983 0.002366 0.028 Uiso 1 1 calc R U . . .
C18 C 0.17992(18) 0.21037(16) 0.10450(12) 0.0151(3) Uani 1 1 d . . . .
S1 S 0.09256(4) 0.34308(4) 0.13369(3) 0.01521(10) Uani 1 1 d . . . .
01 0 -0.01277(14) 0.35697(14) 0.07026(12) 0.0290(3) Uani 1 1 d . . . .
02 0 0.05252(14) 0.32859(13) 0.23374(10) 0.0252(3) Uani 1 1 d . . . .
O3 O 0.18462(13) 0.43560(11) 0.11552(9) 0.0165(3) Uani 1 1 d . . . .
P2 P 0.28115(4) 0.60326(4) 0.30421(3) 0.01297(10) Uani 1 1 d . . .
C21 C 0.24383(19) 0.58697(17) 0.43320(13) 0.0180(4) Uani 1 1 d . . . .
C22 C 0.3306(2) 0.5203(2) 0.48774(15) 0.0278(5) Uani 1 1 d . . . .
H22 H 0.405695 0.484069 0.457496 0.033 Uiso 1 1 calc R U . . .
C23 C 0.3081(3) 0.5063(2) 0.58646(16) 0.0351(5) Uani 1 1 d . . . .
H23 H 0.368419 0.461835 0.623384 0.042 Uiso 1 1 calc R U . . .
C24 C 0.1981(2) 0.5570(2) 0.63029(15) 0.0323(5) Uani 1 1 d . .
H24 H 0.183017 0.547857 0.697551 0.039 Uiso 1 1 calc R U . .
C25 C 0.1096(2) 0.6212(2) 0.57673(16) 0.0354(5) Uani 1 1 d .
H25 H 0.033036 0.654833 0.606923 0.042 Uiso 1 1 calc R U . . .
C26 C 0.1333(2) 0.6364(2) 0.47828(15) 0.0283(5) Uani 1 1 d . . . .
H26 H 0.072902 0.681293 0.441708 0.034 Uiso 1 1 calc R U . . .
C27 C 0.14587(18) 0.69601(16) 0.26284(13) 0.0156(3) Uani 1 1 d . . . .
C28 C 0.0303(2) 0.64407(18) 0.25032(16) 0.0246(4) Uani 1 1 d . . . .
H28 H 0.025388 0.562332 0.259994 0.030 Uiso 1 1 calc R U . . .
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C29 C -0.0774(2) 0.7119(2) 0.22371(17) 0.0309(5) Uani 1 1 d . . . . H29 H -0.156580 0.676679 0.216719 0.037 Uiso 1 1 calc R U . . C30 C -0.0696(2) 0.8308(2) 0.20732(15) 0.0290(5) Uani 1 1 d . . H30 H -0.143575 0.876916 0.189208 0.035 Uiso 1 1 calc R U . . . C31 C 0.0445(2) 0.8822(2) 0.21714(19) 0.0350(5) Uani 1 1 d . . . . H31 H 0.049730 0.963668 0.205219 0.042 Uiso 1 1 calc R U . . . C32 C 0.1527(2) 0.81476(19) 0.24467(18) 0.0289(5) Uani 1 1 d . . . . H32 H 0.231773 0.850464 0.251013 0.035 Uiso 1 1 calc R U . . . C33 C 0.41330(18) 0.70393(16) 0.29692(13) 0.0159(3) Uani 1 1 d . . . . C34 C 0.4303(2) 0.77314(18) 0.37339(14) 0.0236(4) Uani 1 1 d . H34 H 0.378561 0.762419 0.431025 0.028 Uiso 1 1 calc R U . . . C35 C 0.5213(2) 0.8572(2) 0.36677(16) 0.0299(5) Uani 1 1 d . . . H35 H 0.531128 0.903490 0.419548 0.036 Uiso 1 1 calc R U . . . C36 C 0.5976(2) 0.8737(2) 0.28369(17) 0.0286(5) Uani 1 1 d . . . . H36 H 0.658488 0.932494 0.278793 0.034 Uiso 1 1 calc R U . . . C37 C 0.58531(19) 0.80456(17) 0.20749(15) 0.0212(4) Uani 1 1 d . . . . H37 H 0.638661 0.815467 0.150646 0.025 Uiso 1 1 calc R U . . C38 C 0.49505(17) 0.71896(16) 0.21369(13) 0.0144(3) Uani 1 1 d . . . . 021 0 0.59887(14) 0.66422(13) 0.04873(10) 0.0241(3) Uani 1 1 d . . . 022 0 0.36329(14) 0.67175(13) 0.07118(10) 0.0235(3) Uani 1 1 d . . . . 023 0 0.49374(13) 0.51238(11) 0.14302(9) 0.0189(3) Uani 1 1 d . . . . S2 S 0.48665(4) 0.63598(4) 0.11016(3) 0.01485(10) Uani 1 1 d . . . . K1 K 0.24805(4) 0.54177(4) -0.04751(3) 0.01961(9) Uani 1 1 d . . . . loop atom site aniso label atom site aniso U 11 \_atom\_site aniso U 22 \_atom\_site\_aniso U 33 \_atom\_site\_aniso U 23 \_atom\_site aniso U 13 atom site aniso U 12 Cu1 0.01709(12) 0.01060(11) 0.01364(11) -0.00103(8) 0.00038(8) -0.00031(8)P1 0.0153(2) 0.0107(2) 0.0120(2) 0.00015(16) -0.00090(16) -0.00008(16) C1 0.0177(9) 0.0104(8) 0.0246(9) -0.0011(7) -0.0024(7) -0.0008(7) C2 0.0231(10) 0.0171(9) 0.0315(11) 0.0005(8) 0.0036(8) -0.0002(8)C3 0.0222(11) 0.0168(10) 0.0606(16) -0.0035(10) 0.0126(10) -0.0025(8) C4 0.0160(10) 0.0180(10) 0.086(2) -0.0057(12) -0.0085(12) -0.0008(8) C5 0.0283(12) 0.0251(11) 0.0610(16) -0.0015(11) -0.0245(12) -0.0022(9) C6 0.0257(11) 0.0197(10) 0.0305(11) -0.0009(8) -0.0101(9) -0.0024(8) C7 0.0179(9) 0.0188(9) 0.0144(8) 0.0030(7) -0.0016(7) -0.0001(7) C8 0.0429(14) 0.0213(10) 0.0241(10) 0.0004(8) 0.0088(9) 0.0031(9) C9 0.0411(14) 0.0398(13) 0.0218(10) 0.0006(10) 0.0111(9) 0.0127(11) C10 0.0355(13) 0.0437(14) 0.0229(10) 0.0132(10) 0.0070(9) -0.0017(11) C11 0.097(3) 0.0333(14) 0.0315(13) 0.0076(11) 0.0132(15) -0.0261(15) C12 0.086(2) 0.0229(12) 0.0232(11) -0.0004(9) 0.0136(12) -0.0161(13) C13 0.0174(9) 0.0132(8) 0.0132(8) -0.0007(6) 0.0013(6) -0.0027(7)C14 0.0243(10) 0.0151(9) 0.0202(9) -0.0011(7) -0.0013(7) 0.0019(7) C15 0.0388(12) 0.0146(9) 0.0254(10) -0.0075(8) -0.0009(9) 0.0015(8)C16 0.0429(13) 0.0214(10) 0.0226(10) -0.0078(8) -0.0079(9) -0.0041(9) c17 0.0277(11) 0.0213(10) 0.0207(9) -0.0020(8) -0.0062(8) -0.0032(8) C18 0.0176(9) 0.0137(8) 0.0137(8) 0.0004(7) 0.0015(7) -0.0014(7) S1 0.0120(2) 0.0162(2) 0.0174(2) -0.00141(16) -0.00072(16) -0.00010(16) 01 0.0198(8) 0.0287(8) 0.0400(9) -0.0052(7) -0.0142(7) 0.0022(6) 02 0.0248(8) 0.0273(8) 0.0223(7) -0.0024(6) 0.0110(6) -0.0028(6) 03 0.0171(6) 0.0148(6) 0.0172(6) 0.0018(5) -0.0008(5) -0.0003(5) P2 0.0134(2) 0.0125(2) 0.0129(2) -0.00232(16) 0.00178(16) -0.00138(17)

C21 0.0211(9) 0.0184(9) 0.0147(8) -0.0031(7) 0.0032(7) -0.0055(7) C22 0.0274(11) 0.0352(12) 0.0201(10) -0.0012(9) 0.0009(8) 0.0030(9) C23 0.0397(14) 0.0450(14) 0.0203(10) 0.0046(10) -0.0052(9) -0.0017(11) C24 0.0418(14) 0.0410(13) 0.0145(9) -0.0010(9) 0.0049(9) -0.0141(11)C25 0.0337(13) 0.0503(15) 0.0209(10) -0.0052(10) 0.0107(9) -0.0013(11) C26 0.0285(11) 0.0358(12) 0.0193(10) -0.0025(9) 0.0051(8) 0.0032(9) C27 0.0153(9) 0.0163(9) 0.0146(8) -0.0010(7) 0.0032(6) 0.0011(7) C28 0.0196(10) 0.0204(10) 0.0342(11) -0.0060(8) -0.0011(8) -0.0011(8)C29 0.0187(10) 0.0363(12) 0.0383(12) -0.0065(10) -0.0048(9) 0.0000(9) C30 0.0222(11) 0.0381(12) 0.0242(10) 0.0067(9) 0.0022(8) 0.0109(9) C31 0.0301(12) 0.0228(11) 0.0490(14) 0.0129(10) 0.0038(10) 0.0052(9) C32 0.0206(10) 0.0197(10) 0.0453(13) 0.0047(9) 0.0013(9) -0.0018(8) C33 0.0142(8) 0.0166(9) 0.0173(8) -0.0027(7) -0.0015(7) -0.0008(7) C34 0.0256(11) 0.0256(10) 0.0204(9) -0.0084(8) 0.0033(8) -0.0070(8) C35 0.0285(12) 0.0325(12) 0.0311(11) -0.0149(9) -0.0008(9) -0.0114(9) C36 0.0218(10) 0.0258(11) 0.0397(12) -0.0100(9) 0.0014(9) -0.0108(8)C37 0.0154(9) 0.0203(9) 0.0277(10) -0.0021(8) 0.0028(7) -0.0039(7) C38 0.0122(8) 0.0141(8) 0.0170(8) -0.0022(7) -0.0003(6) 0.0002(6) 021 0.0253(8) 0.0227(7) 0.0232(7) -0.0019(6) 0.0131(6) -0.0056(6) 022 0.0226(7) 0.0288(8) 0.0196(7) -0.0036(6) -0.0059(6) 0.0017(6) 023 0.0204(7) 0.0142(6) 0.0213(6) -0.0022(5) 0.0074(5) -0.0014(5) S2 0.0146(2) 0.0156(2) 0.0140(2) -0.00255(16) 0.00322(16) -0.00148(16) K1 0.0193(2) 0.0218(2) 0.01731(19) 0.00169(15) -0.00164(15) 0.00058(16) #\_\_\_\_\_ ---# # MOLECULAR GEOMETRY # #\_\_\_\_\_\_ ---# \_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 \_geom\_bond\_atom\_site\_label 2 geom bond distance \_geom\_bond\_site\_symmetry 2 geom bond publ flag Cul 03 2.1681(13) . ? Cul 023 2.1767(13) . ? Cul P2 2.2195(5) . ? Cu1 P1 2.2278(5) . ? Cul Kl 4.0159(5) . ? P1 C1 1.824(2) . ? P1 C7 1.8267(19) . ? P1 C13 1.8383(19) . ?

C1	С6	1.	396	5 (3	3)	•		2				
C1	C2	1.	401	L (:	3)		5	?				
$C^{2}$	CR	1	29.	1	, 3 )	-		>				
C2	112	⊥ • ∩	050		)	•		•				
	п∠ а ́	∪.	201		•	:		_				
C3	C4	1.	389	) (4	4)	•		2				
C3	K1	3.	393	1(2	2)	2	_ (	56	55	?		
C3	HЗ	0.	950	00		?						
C4	$C_{5}$	1	378	3 (4	4)		-	2				
Сл	цл		050		- /	• ?		•				
	114 a.c	U.	200	, , , ,	•	:		~				
05	C 6	⊥.	394	± (.	3)	•		2				
C5	Н5	0.	950	00	•	?						
C6	НG	0.	950	00		?						
C7	С8	1.	378	3 (3	3)		5	?				
C7	C10	1	29	۲ ۲	, (२	)		2	,			
C 0	C12	, ⊥ 1	201	1 1 1	2 V	/	•	÷				
	(y	⊥.	59.	L (,	ן כ	•						
С8	Н8	υ.	95(	)()	•	?						
С9	C10	1	3	72	(4	)	•	?	•			
С9	Н9	0.	950	00		?						
C10	C1	1	1.	36'	5 (	4)		_	?			
C10	UU1	$\hat{\Box}$	<u> </u>	2 5 ( 2 5 (	- ` \∩	÷ /	-	>	•			
		0	0.	200	) U L	•			0			
CII	. C1	2	⊥.	394	4 (	3)		•	2			
C11	. H1	1	0.9	95(	)0	•		2				
C12	H1	2	0.9	95(	00			?				
C13	C1	4	1.3	398	3 (	3)			?			
C13	C1	8	1 4	100	, ,	31		_	?			
C1 /		5	1	201	- (   /	<i>२</i> ७		•	• ?			
		. J	т.,	ノブ」	⊥ ( \	5)		•	÷			
CI4	H1	4	0.9	95(	00	•		2				
C15	C1	6	1.3	38	7 (	3)		•	?			
C15	H1	5	0.9	950	00			?				
C16	6 C1	7	1.3	391	1 (	3)			?			
C16	; н1	6	0 0	) 5 (	ົ່	'		>	-			
	, 111 , 01	0	1	200	21	2 \ 2 \		•	C			
		Ö	±	200	) C	S)		•	:			
C17	H1	7	0.9	95(	)0	•		Ś				
C18	S1	. 1	78	382	2 (	19	)	•	3	2		
S1	02	1.	445	51	(1	4)			?			
S1	01	1	4.50	)7	(1	، 5١			?			
01	03	• 1	100	,, 1⊑	\⊥ (1	с, л\		•	• ?			
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SI	Κl	J.	694	τŢ	(6	)	•	2	_		-	
01	К1	2.	678	31	(1	5)	2	2_	56	55	?	
03	K1	2.	60'	73	(1	3)			?			
P2	C27	1	. 82	238	3 (	19	)		2	2		
р?	C21	1	2 Q 1	32	- ( 	19	ý	•	-	>		
т <u>с</u>	021	. 1	• U \ •	11		エジ 1 へ	/ \	•	-	>		
rZ	53			±⊥4	± (	тЭ	)	•	:			
C21	C2	6	1.3	384	4 (	3)		•	?			
C21	C2	2	1.3	393	3 (	3)			?			
C22	C2	3	1.3	395	5(	3)			?			
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C23	6 H2	3	υ.	95(	JÜ	•		2				
C24	C2	5	1.3	383	3 (	4)		•	?			
C24	Н2	4	0.9	950	00		5	?				
C25	C.2	6	1	394	4 (	31			?			
C25	U Ц	5	0 0	350	- ` \∩	- /		>	•			
020	, n2		0.3	200	50	•						
C26	) H2	ю	υ.	95(	10	•		-	_			
C27	C3	2	1.3	386	5 (	3)		•	?			
C27	C2	8	1.3	395	5 (	3)			?			
C28	C2	9	1.3	388	3 (	3)			?			
C28	н2	8	0 0	950	ົງດ	- /		>	-			
	· 11乙	0	U • .	~ ~ ~	50	•						

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C29 C30 1.386(3) . ?
C29 H29 0.9500 . ?
C30 C31 1.371(3) . ?
СЗО НЗО 0.9500 . ?
C31 C32 1.394(3) . ?
C31 H31 0.9500 . ?
C32 H32 0.9500 . ?
C33 C34 1.397(3) . ?
C33 C38 1.410(3) . ?
C34 C35 1.387(3) . ?
C34 H34 0.9500 .
                 ?
C35 C36 1.380(3) . ?
C35 H35 0.9500 . ?
C36 C37 1.384(3) . ?
C36 H36 0.9500 . ?
C37 C38 1.395(3) . ?
СЗ7 НЗ7 0.9500 . ?
C38 S2 1.7918(19) . ?
O21 S2 1.4476(14) . ?
021 K1 2.7846(16) 2_665 ?
O22 S2 1.4547(15) . ?
O22 K1 2.6783(15) . ?
O23 S2 1.4760(14) . ?
023 K1 2.9700(14) 2 665 ?
S2 K1 3.4370(6) 2 665 ?
S2 K1 3.6699(6) . ?
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#
# Full information about CCDC data access policies and citation
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on F, with F set to zero for negative F^{2^{-1}}. The threshold expression of
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 $F^2$  > 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  ${\tt F}^2{\tt ^}$  are statistically about twice as large as those based on F, and Rfactors based on ALL data will be even larger. \_refine\_ls\_structure\_factor coef Fsqd refine ls matrix type full calc \_refine\_ls\_weighting\_details  $w=1/[s^2(Fo^2)+(0.0777P)^2+1.1427P]$  where  $P=(Fo^2+2Fc^2)/3$ atom sites solution primary ? ? atom sites solution secondary \_atom\_sites\_solution hydrogens geom \_refine\_ls\_hydrogen\_treatment constr \_\_\_\_\_\_\_refine\_ls\_extinction\_method none \_refine\_ls\_extinction\_coef \_refine\_ls\_number reflns 4806 \_refine\_ls\_number\_parameters 250 \_refine\_ls\_number\_restraints 0 \_refine\_ls\_R\_factor\_all 0.0342 \_refine\_ls R factor gt 0.0297 refine ls wR factor ref 0.1013 refine ls wR factor gt 0.0954 \_refine\_ls\_goodness\_of\_fit ref 0.954 \_refine\_ls\_restrained S all 0.954 \_refine\_ls\_shift/su max 0.002 \_refine\_ls\_shift/su\_mean 0.000 refine diff density max 0.883 refine diff density min -0.535 \_refine\_diff\_density rms 0.123 . . . . . . . # .RES SHELXL file: job.res # .HKL SHELXL file: job.hkl #..... . . . . . . . shelx res file job.res created by SHELXL-2014/7 TITL import a.res in P2(1)/c CELL 0.71073 11.7847 9.0047 20.0552 90.000 97.723 90.000 4.00 0.0004 0.0003 0.0007 0.000 0.001 0.000 ZERR LATT 1 - X, 1/2 + Y, 1/2 - ZSYMM H P CU 104 4 4 0 SFAC C Η S 20 76 UNIT 4 MERG 2 FMAP 2 20 PLAN ACTA

BOND \$H CONF LIST 4 WPDB -2 L.S. 4 TEMP -123.00 WGHT 0.077700 1.142700 FVAR 0.68607 CU1 4 0.437510 0.317427 0.664802 11.00000 0.01074 0.01627 =0.01417 0.00069 -0.00083 0.00270 0.273496 0.397135 0.616434 11.00000 0.00856 P1 3 0.00853 =0.00988 0.00095 0.00076 -0.00039 5 0.585392 0.431796 0.699691 11.00000 0.01245 01 0.01937 =0.04753 -0.01190 -0.00129 -0.00099 0.698981 0.387938 0.691304 11.00000 C2 1 0.01600 0.02428 =0.04105 -0.00387 0.00433 -0.00135 AFIX 137 11.00000-1.5000011.00000-1.5000011.00000-1.50000 H2A 2 0.713416 0.287255 0.708983 2 0.753971 0.456826 0.715792 H2B 2 H2C 0.707559 0.389616 0.643378 AFIX 0 011 5 11.00000 0.525938 0.123044 0.645894 0.02399 0.01816 =0.01960 -0.00559 -0.00210 0.00872 0.551283 0.072100 0.582160 11.00000 0.02284 C12 1 0.03750 =0.02144 -0.00560 0.00252 0.01155 AFIX 137 H12A 2 0.480768 0.037396 0.555166 11.00000 -1.50000 0.606411 -0.009786 0.588884 H12B 2 11.00000 -1.5000011.00000 H12C 2 0.584078 0.153701 0.558658 -1.50000AFIX 0 1 C21 0.254267 0.362724 0.523026 11.00000 0.01219 0.01551 =0.01066 0.00129 0.00198 0.00022 1 0.245254 0.194622 0.510359 11.00000 0.02284 C22 0.01706 =0.01504 -0.00436 0.00529 0.00019 AFTX 137 H22A 2 0.169021 0.160003 0.517599 11.00000 -1.50000H22B 2 0.303535 0.143197 0.541476 -1.50000 11.00000 H22C 2 0.257455 0.173427 0.463923 11.00000 -1.50000 AFIX 0 1 0.367178 0.419105 0.500776 11.00000 C23 0.01697 0.02865 =0.01636 0.00334 0.00638 -0.00338 AFIX 137 H23A 2 0.366002 0.525818 11.00000 0.431945 -1.50000 H23B 2 0.525768 0.375212 0.509916 11.00000 -1.50000 H23C 2 0.365998 0.401306 0.452481 11.00000 -1.50000 AFIX 0 C24 1 0.156350 0.445523 0.480531 11.00000 0.01669 0.02694 =0.01330 0.00441 -0.00130 0.00334

AFIX 137 0.1596620.4265590.43271311.00000-1.500000.1639350.5523450.48936711.00000-1.500000.0828490.4106020.49234111.00000-1.50000 H24A 2 H24B 2 H24C 2 AFIX 0 0.623795 11.00000 C25 0.241367 0.594143 0.01732 1 0.00887 =0.01216 0.00153 0.00191 -0.00007 C26 1 0.129366 0.646750 0.620556 11.00000 0.01994 0.01449 =0.02225 0.00090 0.00334 0.00229 AFIX 43 0.067190 0.578716 0.615591 11.00000 -1.20000 H26 2 AFIX 0 C27 1 0.108242 0.798543 0.624566 11.00000 0.03208 0.01797 = 0.03009 0.00375 0.00922 0.01123 AFIX 43 H27 2 0.031853 0.833960 0.622072 11.00000 -1.20000 AFIX 0 1 C28 0.198195 0.896757 0.632133 11.00000 0.04914 0.01030 = 0.03133 0.00179 0.01120 0.00534 AFIX 43 H28 2 0.183536 1.000223 0.634558 11.00000 -1.20000 AFIX O C29 1 0.309971 0.846731 0.636268 11.00000 0.04313 0.01393 =0.03793 -0.00110 0.00808 -0.01069 AFIX 43 H29 2 0.371612 0.915557 0.641913 11.00000 -1.20000 AFIX O C30 1 0.331892 0.695105 0.632130 11.00000 0.02062 0.01535 =0.02661 0.00103 0.00232 -0.00466 AFIX 43 Н30 2 0.408556 0.660537 0.634991 11.00000 -1.20000 AFIX 0 C31 1 0.156270 0.306610 0.653414 11.00000 0.01178 0.00869 =0.01200 -0.00050 0.00372 0.00009 c32 1 0.054533 0.263467 0.613770 11.00000 0.01273 0.01112 = 0.01596 -0.00030 0.00238 -0.00044 AFIX 43 2 0.043757 0.289182 0.567409 11.00000 -1.20000 Н32 AFIX 0 1 -0.031964 0.183957 0.639692 11.00000 0.01250 C33 0.01280 =0.02687 -0.00382 0.00455 -0.00262 C34 1 -0.018221 0.152868 0.707906 11.00000 0.01804 0.02033 = 0.02914 0.00297 0.01129 -0.00500 AFIX 43 Н34 2 -0.076659 0.101269 0.726727 11.00000 -1.20000 AFIX 0 C35 1 0.080340 0.196579 0.748962 11.00000 0.01975 0.02144 =

0.01830 0.00257 0.00833 -0.00110 AFIX 43 Н35 2 0.088093 0.175898 0.795805 11.00000 -1.20000 AFIX 0 C36 1 0.168105 0.270367 0.722477 11.00000 0.01451 0.01096 = 0.01289 -0.00088 0.00341 0.00097 C37 1 -0.136065 0.132846 0.592953 11.00000 0.01562 0.02859 =0.03540 -0.00406 0.00200 -0.00882 AFIX 137 H37A2-0.1769290.0571430.61553911.00000-1.50000H37B2-0.1118560.0906600.55208311.00000-1.50000H37C2-0.1868790.2176090.58094611.00000-1.50000 AFIX O si 6 0.292991 0.313915 0.780514 11.00000 0.01894 0.01338 = 0.00917 0.00000 0.00074 -0.00060 038 5 0.312082 0.472485 0.772343 11.00000 0.02727 0.01357 =0.01842 -0.00258 -0.00337 -0.00258 5 0.267259 0.271526 0.846351 11.00000 0.03239 039 0.03009 = 0.01053 0.00188 0.00452 -0.00148 040 5 0.387451 0.224655 0.759662 11.00000 0.01714 0.01707 =0.01623 0.00421 0.00083 0.00262 HKLF 4 REM import a.res in P2(1)/c REM R1 = 0.0297 for 4339 Fo > 4sig(Fo) and 0.0342 for all 4806 data REM 250 parameters refined using 0 restraints END 0.0488 1.3012 WGHT REM Highest difference peak 0.883, deepest hole -0.535, 1-sigma level 0.123 Q1 1 0.5863 0.5244 0.7086 11.00000 0.05 0.88 1 0.2509 0.2772 0.5204 11.00000 0.05 0.47 Q2 1 0.1197 0.7262 0.6276 11.00000 0.05 0.46 Q3 1 0.2994 0.4063 0.7740 11.00000 0.05 0.45 Q4 0.5716 0.0765 0.6783 11.00000 0.05 0.3602 0.2731 0.6173 11.00000 0.05 Q5 1 0.44 06 0.39 1 1 0.4596 0.2657 0.6127 11.00000 0.05 0.38 Q7 0.38 1 0.2553 0.5205 0.6219 11.00000 0.05 Q8 Q.9 1 0.1853 0.5808 0.4644 11.00000 0.05 0.36 Q10 1 0.3390 0.3060 0.6437 11.00000 0.05 0.35 1 -0.0868 0.1383 0.6131 11.00000 0.05 0.34 Q11 0.5020 -0.0953 0.6027 11.00000 0.05 0.34 Q12 1 1 -0.1172 0.0561 0.5936 11.00000 0.05 0.33 Q13 
 1
 0.4543
 0.5836
 0.5787
 11.00000
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 1
 0.1990
 0.3321
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 014 0.32 1 0.31 015 0.31 Q16 1 -0.0050 0.7766 0.6041 11.00000 0.05 1 0.5035 0.1979 0.6526 11.00000 0.05 0.31 Q17 Q18 1 0.2227 0.4168 0.7393 11.00000 0.05 0.31

Q19 1 0.0578 0.4219 0.6893 11.00000 0.05 0.30 Q20 1 0.1485 0.4269 0.6923 11.00000 0.05 0.30 shelx res checksum 94844 # ..... End of .HKL file #\_\_\_\_\_\_ ---# ---# # ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS # #\_\_\_\_\_\_ ---# loop\_ atom type symbol \_atom\_type\_description \_atom\_type\_scat\_dispersion real \_atom\_type\_scat\_dispersion imag \_atom\_type scat source C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' P P 0.1023 0.0942 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' Cu Cu 0.3201 1.2651 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' 0 0 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' loop atom site label atom site type symbol \_atom\_site\_fract x \_atom\_site\_fract\_y \_atom\_site\_fract\_z \_atom\_site U iso or equiv \_atom\_site\_adp type atom site occupancy atom site site symmetry order atom site calc flag \_atom\_site\_refinement\_flags posn \_atom\_site\_refinement\_flags\_adp \_atom\_site\_refinement\_flags\_occupancy \_atom\_site\_disorder assembly atom site disorder group Cu1 Cu 0.43751(2) 0.31743(2) 0.66480(2) 0.01396(9) Uani 1 1 d . . . . P1 P 0.27350(3) 0.39713(4) 0.61643(2) 0.00903(11) Uani 1 1 d . . . . O1 O 0.58539(11) 0.43180(15) 0.69969(8) 0.0269(3) Uani 1 1 d . . . . C2 C 0.69898(16) 0.3879(2) 0.69130(12) 0.0271(4) Uani 1 1 d . . . . H2A H 0.7134 0.2873 0.7090 0.041 Uiso 1 1 calc R U . . . H2B H 0.7540 0.4568 0.7158 0.041 Uiso 1 1 calc R U . . . H2C H 0.7076 0.3896 0.6434 0.041 Uiso 1 1 calc R U . . . 011 0 0.52594(12) 0.12304(14) 0.64589(7) 0.0210(3) Uani 1 1 d . . . . C12 C 0.55128(17) 0.0721(3) 0.58216(10) 0.0273(4) Uani 1 1 d . . . . H12A H 0.4808 0.0374 0.5552 0.041 Uiso 1 1 calc R U . . .

H12B H 0.6064 -0.0098 0.5889 0.041 Uiso 1 1 calc R U . . . H12C H 0.5841 0.1537 0.5587 0.041 Uiso 1 1 calc R U . . . C21 C 0.25427(14) 0.36272(19) 0.52303(8) 0.0127(3) Uani 1 1 d . . . . C22 C 0.24525(17) 0.19462(19) 0.51036(10) 0.0181(4) Uani 1 1 d . . . . H22A H 0.1690 0.1600 0.5176 0.027 Uiso 1 1 calc R U . . . H22B H 0.3035 0.1432 0.5415 0.027 Uiso 1 1 calc R U . . . H22C H 0.2575 0.1734 0.4639 0.027 Uiso 1 1 calc R U . . . C23 C 0.36718(15) 0.4191(2) 0.50078(9) 0.0203(4) Uani 1 1 d . . . . H23A H 0.4319 0.3660 0.5258 0.030 Uiso 1 1 calc R U . . . H23B H 0.3752 0.5258 0.5099 0.030 Uiso 1 1 calc R U . . H23C H 0.3660 0.4013 0.4525 0.030 Uiso 1 1 calc R U . . . C24 C 0.15635(15) 0.4455(2) 0.48053(9) 0.0193(4) Uani 1 1 d . . . . H24A H 0.1597 0.4266 0.4327 0.029 Uiso 1 1 calc R U . . . H24B H 0.1639 0.5523 0.4894 0.029 Uiso 1 1 calc R U . . . H24C H 0.0828 0.4106 0.4923 0.029 Uiso 1 1 calc R U . . . C25 C 0.24137(14) 0.59414(18) 0.62379(8) 0.0128(3) Uani 1 1 d . . . . C26 C 0.12937(16) 0.6467(2) 0.62056(9) 0.0188(4) Uani 1 1 d . . . . H26 H 0.0672 0.5787 0.6156 0.023 Uiso 1 1 calc R U . . . C27 C 0.10824(19) 0.7985(2) 0.62457(11) 0.0263(4) Uani 1 1 d . . . H27 H 0.0319 0.8340 0.6221 0.032 Uiso 1 1 calc R U . . . C28 C 0.1982(2) 0.8968(2) 0.63213(11) 0.0297(5) Uani 1 1 d . . . . H28 H 0.1835 1.0002 0.6346 0.036 Uiso 1 1 calc R U . . . C29 C 0.3100(2) 0.8467(2) 0.63627(12) 0.0314(5) Uani 1 1 d . . . . H29 H 0.3716 0.9156 0.6419 0.038 Uiso 1 1 calc R U . . . C30 C 0.33189(17) 0.6951(2) 0.63213(11) 0.0209(4) Uani 1 1 d . . . . H30 H 0.4086 0.6605 0.6350 0.025 Uiso 1 1 calc R U . . . C31 C 0.15627(14) 0.30661(16) 0.65341(9) 0.0106(3) Uani 1 1 d . . . . C32 C 0.05453(14) 0.26347(18) 0.61377(9) 0.0132(3) Uani 1 1 d . . . . H32 H 0.0438 0.2892 0.5674 0.016 Uiso 1 1 calc R U . . . C33 C -0.03196(15) 0.18396(18) 0.63969(10) 0.0172(4) Uani 1 1 d . . . . C34 C -0.01822(16) 0.1529(2) 0.70791(11) 0.0218(4) Uani 1 1 d . . . . H34 H -0.0767 0.1013 0.7267 0.026 Uiso 1 1 calc R U . . . C35 C 0.08034(16) 0.1966(2) 0.74896(10) 0.0193(4) Uani 1 1 d . . . . H35 H 0.0881 0.1759 0.7958 0.023 Uiso 1 1 calc R U . . C36 C 0.16810(14) 0.27037(18) 0.72248(8) 0.0126(3) Uani 1 1 d . . . . C37 C -0.13607(16) 0.1328(2) 0.59295(11) 0.0267(4) Uani 1 1 d . . . . H37A H -0.1769 0.0571 0.6155 0.040 Uiso 1 1 calc R U . . . H37B H -0.1119 0.0907 0.5521 0.040 Uiso 1 1 calc R U . . . H37C H -0.1869 0.2176 0.5809 0.040 Uiso 1 1 calc R U . . . S1 S 0.29299(4) 0.31392(4) 0.78051(2) 0.01394(11) Uani 1 1 d . . . . O38 O 0.31208(12) 0.47249(14) 0.77234(7) 0.0203(3) Uani 1 1 d . . . . 039 0 0.26726(13) 0.27153(17) 0.84635(7) 0.0242(3) Uani 1 1 d . . . . 040 0 0.38745(11) 0.22465(14) 0.75966(6) 0.0169(3) Uani 1 1 d . . . . loop\_ \_atom\_site\_aniso\_label \_atom\_site\_aniso U 11 atom site aniso U 22 atom site aniso U 33 atom site aniso U 23 atom site aniso U 13 atom site aniso U 12 Cul 0.01074(13) 0.01627(14) 0.01417(14) 0.00069(7) -0.00083(9) 0.00270(7) P1 0.00856(19) 0.00853(19) 0.0099(2) 0.00095(14) 0.00076(14) -0.00039(13) 01 0.0124(6) 0.0194(7) 0.0475(9) -0.0119(6) -0.0013(6) -0.0010(5) C2 0.0160(9) 0.0243(10) 0.0411(12) -0.0039(8) 0.0043(8) -0.0013(7) 011 0.0240(7) 0.0182(6) 0.0196(7) -0.0056(5) -0.0021(5) 0.0087(5) C12 0.0228(9) 0.0375(11) 0.0214(10) -0.0056(8) 0.0025(7) 0.0116(8)

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C21 0.0122(7) 0.0155(8) 0.0107(7) 0.0013(6) 0.0020(6) 0.0002(6)
C22 0.0228(9) 0.0171(8) 0.0150(9) -0.0044(6) 0.0053(7) 0.0002(6)
C23 0.0170(8) 0.0287(9) 0.0164(9) 0.0033(7) 0.0064(7) -0.0034(7)
C24 0.0167(8) 0.0269(9) 0.0133(8) 0.0044(7) -0.0013(6) 0.0033(7)
\texttt{C25 0.0173(8) 0.0089(7) 0.0122(7) 0.0015(6) 0.0019(6) -0.0001(6)}
C26 0.0199(9) 0.0145(8) 0.0222(9) 0.0009(7) 0.0033(7) 0.0023(7)
C27 0.0321(11) 0.0180(9) 0.0301(11) 0.0037(8) 0.0092(9) 0.0112(8)
C28 0.0491(13) 0.0103(8) 0.0313(11) 0.0018(7) 0.0112(10) 0.0053(8)
C29 0.0431(13) 0.0139(8) 0.0379(12) -0.0011(8) 0.0081(10) -0.0107(8)
C30 0.0206(9) 0.0153(8) 0.0266(10) 0.0010(7) 0.0023(7) -0.0047(6)
C31 0.0118(7) 0.0087(7) 0.0120(8) -0.0005(5) 0.0037(6) 0.0001(5)
C32 0.0127(7) 0.0111(7) 0.0160(8) -0.0003(6) 0.0024(6) -0.0004(6)
C33 0.0125(8) 0.0128(8) 0.0269(10) -0.0038(6) 0.0045(7) -0.0026(6)
C34 0.0180(9) 0.0203(8) 0.0291(10) 0.0030(8) 0.0113(7) -0.0050(7)
C35 0.0197(9) 0.0214(9) 0.0183(9) 0.0026(7) 0.0083(7) -0.0011(7)
C36 0.0145(7) 0.0110(7) 0.0129(8) -0.0009(6) 0.0034(6) 0.0010(6)
C37 0.0156(9) 0.0286(10) 0.0354(12) -0.0041(9) 0.0020(8) -0.0088(8)
S1 0.0189(2) 0.0134(2) 0.0092(2) 0.00000(13) 0.00074(16) -0.00060(14)
038 0.0273(7) 0.0136(6) 0.0184(6) -0.0026(5) -0.0034(5) -0.0026(5)
039 0.0324(8) 0.0301(7) 0.0105(6) 0.0019(5) 0.0045(5) -0.0015(6)
040 0.0171(6) 0.0171(6) 0.0162(6) 0.0042(5) 0.0008(5) 0.0026(5)
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                              MOLECULAR GEOMETRY
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_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
_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry 2
geom bond publ flag
Cul Ol 2.0639(13) . ?
Cu1 011 2.0975(13) . ?
Cul Pl 2.1652(4) . ?
Cul 040 2.2286(13) . ?
P1 C25 1.8241(16) . ?
P1 C31 1.8435(17) . ?
P1 C21 1.8822(17) . ?
O1 C2 1.427(2) . ?
C2 H2A 0.9800 . ?
C2 H2B 0.9800 . ?
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C2 F 011 C12 C12 C21 C21 C21 C21 C22 C22 C22 C	I2C 0 C12 H12A H12B H12C C24 C22 C23 H22A H22B H22C H23A H22B H22C H23A H22B H23A H24B H23C C26 C27 H26 C27 H26 C29 H28 C30 H29 H30 C32 C33 H32 C35 H34 C35 S1 1 H37A H37B	.9800 .9800 1.427 0.98 0.98 0.98 1.533 1.533 1.545 0.98 0.95	0       .         7 (2)         300         300         300         300         300         300         300         5 (2)         5 (2)         5 (2)         5 (2)         5 (2)         300         4 (3)         200         2 (2)         2 (2)         2 (2)         2 (2)         2 (2)         2 (2)         2 (2)         2 (2)         3 (2)         3 (2)         3 (2)         3 (2)         3 (2)         3 (2)	··(。。。。。。。。。。。。。。。。。。。。。。。。。。。。。。。。。。。	
C36 C37 C37 C37 S1 C S1 C S1 C	S1 1 H37A H37B H37C 39 1 38 1 38 1	.7928 0.98 0.98 .4452 .4582 .4782	3 (17 300 300 2 (14 2 (13 2 (13	) . ?	
loop _geo _geo _geo _geo _geo 01 0 01 0 01 0	oan oman oman oman oman oman cul_O Cul_P Cul_Cul_Cul_Cul_O	gle_a gle_a gle_s gle_s gle_s gle_s gle_p 11 93 1 130 P1 12	atom atom site site oubl 3.46 ).45 29.1 )1.8	_site_ _site_ _site_ _symme _flag (5) . (4) . 2(4) . 9(6) .	_label_1 _label_2 _label_3 etry_1 etry_3 .? .? .?

O11 Cu1 O40 92.09(5) . . ? P1 Cu1 O40 100.60(3) . . ? C25 P1 C31 102.86(7) . . ? C25 P1 C21 104.01(8) . . ? C31 P1 C21 109.34(7) . . ? C25 P1 Cu1 117.95(6) . . ? C31 P1 Cu1 110.20(5) . . ? C21 P1 Cu1 111.85(5) . . ? C2 O1 Cu1 125.78(12) . . ? O1 C2 H2A 109.5 . . ? O1 C2 H2B 109.5 . . ? H2A C2 H2B 109.5 . . ? O1 C2 H2C 109.5 . . ? H2A C2 H2C 109.5 . . ? H2B C2 H2C 109.5 . . ? C12 O11 Cu1 126.81(12) . . ? O11 C12 H12A 109.5 . . ? O11 C12 H12B 109.5 . . ? H12A C12 H12B 109.5 . . ? O11 C12 H12C 109.5 . . ? H12A C12 H12C 109.5 . . ? H12B C12 H12C 109.5 . . ? C24 C21 C22 110.93(14) . . ? C24 C21 C23 107.03(14) . . ? C22 C21 C23 108.61(15) . . ? C24 C21 P1 117.02(12) . . ? C22 C21 P1 108.86(12) . . ? C23 C21 P1 103.90(11) . . ? C21 C22 H22A 109.5 . . ? C21 C22 H22B 109.5 . . ? H22A C22 H22B 109.5 . . ? C21 C22 H22C 109.5 . . ? H22A C22 H22C 109.5 . . ? H22B C22 H22C 109.5 . . ? C21 C23 H23A 109.5 . . ? C21 C23 H23B 109.5 . . ? H23A C23 H23B 109.5 . . ? C21 C23 H23C 109.5 . . ? H23A C23 H23C 109.5 . . ? H23B C23 H23C 109.5 . . ? C21 C24 H24A 109.5 . . ? C21 C24 H24B 109.5 . . ? H24A C24 H24B 109.5 . . ? C21 C24 H24C 109.5 . . ? H24A C24 H24C 109.5 . . ? H24B C24 H24C 109.5 . . ? C30 C25 C26 119.20(16) . . ? C30 C25 P1 118.68(13) . . ? C26 C25 P1 122.12(13) . . ? C27 C26 C25 120.36(18) . . ? C27 C26 H26 119.8 . . ? C25 C26 H26 119.8 . . ? C28 C27 C26 119.79(19) . . ? C28 C27 H27 120.1 . . ? C26 C27 H27 120.1 . . ? C27 C28 C29 120.76(18) . . ? C27 C28 H28 119.6 . . ? C29 C28 H28 119.6 . . ?

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C28 C29 C30 119.8(2) . . ?
C28 C29 H29 120.1 . . ?
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H37B C37 H37C 109.5 . . ?
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O38 S1 C36 105.47(8) . . ?
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039 S1 040 Cu1 -172.20(7) . . . ?
O38 S1 O40 Cu1 -42.36(9) . . . ?
C36 S1 O40 Cu1 72.13(8) . . . ?
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# This file contains crystal structure data downloaded from the
# Cambridge Structural Database (CSD) hosted by the Cambridge
# Crystallographic Data Centre (CCDC).
#
# Full information about CCDC data access policies and citation
# guidelines are available at http://www.ccdc.cam.ac.uk/access/V1
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# Audit and citation data items may have been added by the CCDC.
# Please retain this information to preserve the provenance of
# this file and to allow appropriate attribution of the data.
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'-x, -y, -z'
'x, -y-1/2, z-1/2'
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_cell_length_c
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cell volume
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\_cell\_formula\_units\_Z 4 \_cell\_measurement\_temperature150(2)\_cell\_measurement\_reflns\_used9734\_cell\_measurement\_theta\_min2.55\_cell\_measurement\_theta\_max27.47\_cell\_measurement\_wavelength0.71073 ---# # CRYSTAL INFORMATION # ---# \_exptl\_crystal\_description prism colourless 0.600 0.590 exptl\_crystal\_colour \_exptl\_crystal\_size\_max \_exptl\_crystal\_size\_mid \_exptl\_crystal\_size\_min 0.160 \_exptl\_crystal\_density\_meas ? \_exptl\_crystal\_density\_method ? \_exptl\_crystal F 000 1176 \_exptl\_special details ; ? ; ---# # ABSORPTION CORRECTION # #--------# \_exptl\_absorpt\_coefficient\_mu 0.982
\_exptl\_absorpt\_correction\_type multi-scan \_exptl\_absorpt\_process\_details ; [Sheldrick, G.M. (2014). SADABS Bruker AXS Inc., Madison, Wisconsin, USA] ; exptl absorpt correction T min 0.581 exptl absorpt correction T max 0.855 #\_\_\_\_\_ \_\_\_\_\_ ---# # DATA COLLECTION # ---# \_diffrn\_measurement\_device\_type 'D8 VENTURE Bruker AXS' \_diffrn\_measurement\_method 'rotation images' diffrn\_detector '(CMOS) PHOTON 100' \_diffrn\_detector diffrn radiation type MoK∖a

diffrn radiation probe \_\_\_\_\_\_diffrn\_radiation\_source x-ray 'Incoatec microfocus sealed tube' \_diffrn\_radiation\_monochromator 'multilayer monochromator' \_diffrn\_reflns\_av\_r\_equivalents 0.0466 \_diffrn\_reflns\_av\_uneti/neti 0.0429 31421 diffrn reflns number \_diffrn\_reflns limit h min -21 diffrn reflns limit h max 21 -11 \_diffrn\_reflns\_limit\_k\_max 11 \_diffrn\_reflns\_limit\_l\_min \_diffrn\_reflns\_limit\_l\_max -23 24 2.992 \_diffrn\_reflns\_theta min 27.478 diffrn reflns theta max diffrn reflns theta full 25.242 diffrn measured fraction theta full 0.998 \_diffrn\_measured\_fraction\_theta\_max 0.998 \_reflns\_number\_total 6180 \_reflns\_number\_gt 5297 reflns threshold expression >2sigma(I) #\_\_\_\_\_\_ ---# # COMPUTER PROGRAMS USED # ---# \_computing\_data\_collection 'SAINT (Bruker, 2014)'
\_computing\_cell\_refinement 'APEX3 (Bruker, 2015); 'APEX3 (Bruker, 2015); SAINT (Bruker, 2014)' \_computing\_data\_reduction 'SAINT (Bruker, 2014)'
\_computing\_structure\_solution 'SIR97 (Altomare et al., 1999)' \_computing\_structure\_refinement 'SHELXL-2014/7 (Sheldrick, 2014)' computing molecular graphics 'SXGRAPH (Farrugia, 1999), Mercury (CSD, 2014)' computing publication material 'CRYSCALC (T. Roisnel, local program, 2016)' #\_\_\_\_\_ ---# # REFINEMENT INFORMATION # #--------# \_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  $F^2$  > 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  $F^{2^{-1}}$  are statistically about twice as large as those based on F, and Rfactors based on ALL data will be even larger.

; \_refine\_ls\_structure\_factor\_coef Fsqd \_refine\_ls\_matrix\_type full \_refine\_ls\_weighting\_scheme calc refine ls weighting details  $w=1/[s^2(Fo^2)+(0.0261P)^2+2.1854P]$  where  $P=(Fo^2+2Fc^2)/3$ \_atom\_sites\_solution\_primary ? atom sites solution secondary ? atom sites solution hydrogens geom \_refine\_ls\_hydrogen\_treatment constr \_\_\_\_\_\_refine\_ls\_extinction\_method none \_refine\_ls\_extinction\_coef \_refine\_ls\_number\_reflns 6180 329 \_refine\_ls\_number\_parameters \_refine\_ls\_number\_restraints 0 \_refine\_ls\_R\_factor all 0.0416 \_refine\_ls\_R\_factor\_gt 0.0326 \_refine\_ls\_wR\_factor\_ref 0.0837 \_refine\_ls\_wR\_factor\_gt 0.0788 \_refine\_ls\_goodness\_of\_fit\_ref 1.037 \_refine\_ls\_restrained\_S\_all 1.037 \_refine\_ls\_shift/su max 0.002 \_refine\_ls\_shift/su mean 0.000 \_refine\_diff\_density max 0.540 refine diff density min -0.572 refine diff density rms 0.068 \_shelx\_res\_file ; .res SHELXL file: MACu1ACN.res #\_\_\_\_\_ MACulACN.res created by SHELXL-2014/7 TITL import\_a.res in P2(1)/c CELL 0.71073 16.5089 8.8665 19.1633 90.000 106.257 90.000 4.00 0.0022 ZERR 0.0012 0.0021 0.000 0.004 0.000 LATT 1 SYMM - X, 1/2 + Y, 1/2 - ZSFAC C H CU P N 0 S UNIT 104 104 4 4 16 12 4 MERG 2 FMAP 2 PLAN 20 0.16 0.59 0.60 SIZE ACTA BOND \$Н CONF LIST 4 WPDB -2 4 L.S. TEMP -123.00 WGHT 0.026100 2.185400 0.47963 FVAR 1 MOLE CU1 3 0.221029 0.248394 0.578946 11.00000 0.01443 0.02111 = 0.01995 -0.00067 0.00421 0.00510

0.333343 0.157232 0.552663 11.00000 Р1 4 0.01096 0.01266 = 0.01380 -0.00135 0.00216 0.00074 0.236851 -0.080588 0.635437 11.00000 7 0.01405 S1 0.01906 =0.01715 0.00186 0.00407 -0.00119 6 0.306623 -0.007661 0.687065 11.00000 0.01822 01 0.02825 =0.01732 -0.00121 0.00082 -0.00184 02 6 0.205635 -0.214737 0.662709 11.00000 0.02972 0.02498 =0.03021 0.00446 0.01337 -0.00570 6 0.168163 0.025723 0.602120 11.00000 0.01326 03 0.02782 =0.02349 0.00240 0.00488 0.00390 5 0.215520 0.373723 0.663835 11.00000 N1 0.02198 0.02644 =0.02394 -0.00148 0.00488 0.00471 5 0.115819 0.308269 0.503438 11.00000 0.02399 N2 0.03183 =0.02519 -0.00104 0.00184 0.00873 1 0.359632 0.242591 0.474724 11.00000 0.01800 C10.01185 = 0.01560 -0.00072 0.00488 0.00157 C2 1 0.294481 0.262097 0.410344 11.00000 0.01893 0.01825 =0.01951 -0.00190 0.00140 0.00175 AFIX 43 0.238674 0.231563 0.408186 11.00000 -1.20000 Н2 2 AFIX 0 C3 1 0.311347 0.325951 0.349726 11.00000 0.03090 0.02091 =0.01727 0.00072 0.00130 0.00461 AFIX 43 H.3 0.267191 0.336705 0.305923 11.00000 -1.20000 2 AFIX 0 1 0.392362 C4 0.374269 0.352646 11.00000 0.03804 0.02298 =0.02157 0.00556 0.01157 0.00053 AFIX 43 H4 2 0.403602 0.417850 0.311033 11.00000 -1.20000 AFIX 0 C5 1 0.456436 0.358479 0.416490 11.00000 0.02686 0.02982 = 0.02763 0.00509 0.00956 -0.00512 AFIX 43 2 Н5 0.511676 0.392875 0.418989 11.00000 -1.20000 AFIX 0 С6 1 0.440285 0.292169 0.477322 11.00000 0.01916 0.02312 =0.01907 0.00350 0.00354 -0.00096 AFIX 43 2 0.484796 0.280851 0.520844 11.00000 -1.20000 Hб AFIX 0 C11 1 0.433908 0.155481 0.622790 11.00000 0.01398 0.01637 =0.01237 0.00090 0.00369 -0.00158

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 Q2 0.38 Q3 0.35 1 0.2249 0.3404 0.5585 11.00000 0.05 Q4 0.34 1 0.0987 0.9418 0.4246 11.00000 0.05 0.34 Q5 Q6 1 0.2585 -0.2063 0.5439 11.00000 0.05 0.34 1 0.2275 0.1406 0.6079 11.00000 0.05 Q7 0.34 1 0.2613 -0.1090 0.5885 11.00000 0.05 0.34 Q8 0.3388 0.2251 0.5193 11.00000 0.05 0.33 Q.9 1 0.2203 0.1650 0.5510 11.00000 0.05 Q10 1 0.31 1 0.0740 0.2604 0.2576 11.00000 0.05 0.30 011 1 0.3308 -0.0729 0.4983 11.00000 0.05 0.29 Q12 1 0.2280 -0.1532 0.6578 11.00000 0.05 0.29 Q13 Q14 1 0.4441 0.2254 0.6400 11.00000 0.05 0.29 1 0.3344 -0.1794 0.4705 11.00000 0.05 0.29 015 1 0.3463 0.1829 0.5007 11.00000 0.05 0.28 Q16 1 -0.0404 0.3117 0.3684 11.00000 0.05 0.28 Q17 1 0.4568 0.0854 0.6370 11.00000 0.05 0.28 Q18 1 0.3934 0.2957 0.4787 11.00000 0.05 0.27 Q19 Q20 1 0.0508 0.8407 0.4365 11.00000 0.05 0.27 ; shelx res checksum 17866 # ..... End of .RES file # # .HKL SHELXL file: MACu1ACN.hkl # #\_\_\_\_\_\_ ---# #\_\_\_\_\_ ---# # ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS # #\_\_\_\_\_\_ ---# loop\_ atom type symbol \_atom\_type\_description \_atom\_type\_scat\_dispersion\_real \_atom\_type\_scat\_dispersion\_imag atom type scat source C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

Cu Cu 0.3201 1.2651 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' P P 0.1023 0.0942 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' 0 0 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' loop atom site label atom site type symbol \_atom\_site\_fract x \_atom\_site\_fract\_y \_atom\_site\_fract\_z atom site U iso or equiv \_atom\_site\_adp\_type \_atom\_site occupancy \_atom\_site\_site\_symmetry\_order atom site calc flag \_atom\_site\_refinement flags posn \_atom\_site\_refinement\_flags\_adp \_atom\_site\_refinement\_flags occupancy atom site disorder assembly atom site disorder group Cu1 Cu 0.22103(2) 0.24839(2) 0.57895(2) 0.01862(7) Uani 1 1 d . . . . P1 P 0.33334(3) 0.15723(5) 0.55266(2) 0.01274(9) Uani 1 1 d . . . . S1 S 0.23685(3) -0.08059(5) 0.63544(2) 0.01681(10) Uani 1 1 d . . . . 01 0 0.30662(8) -0.00766(15) 0.68706(7) 0.0221(3) Uani 1 1 d . . . . 02 0 0.20564(9) -0.21474(16) 0.66271(8) 0.0273(3) Uani 1 1 d . . . O3 O 0.16816(8) 0.02572(15) 0.60212(7) 0.0216(3) Uani 1 1 d . . . . N1 N 0.21552(10) 0.37372(19) 0.66383(9) 0.0244(3) Uani 1 1 d . . . . N2 N 0.11582(11) 0.3083(2) 0.50344(9) 0.0280(4) Uani 1 1 d . . . . C1 C 0.35963(11) 0.24259(18) 0.47472(9) 0.0151(3) Uani 1 1 d . . . . C2 C 0.29448(12) 0.2621(2) 0.41034(10) 0.0197(4) Uani 1 1 d . . . . H2 H 0.2387 0.2316 0.4082 0.024 Uiso 1 1 calc R U . . C3 C 0.31135(13) 0.3260(2) 0.34973(10) 0.0241(4) Uani 1 1 d . . . H3 H 0.2672 0.3367 0.3059 0.029 Uiso 1 1 calc R U . . C4 C 0.39236(14) 0.3743(2) 0.35265(11) 0.0269(4) Uani 1 1 d . . . . H4 H 0.4036 0.4178 0.3110 0.032 Uiso 1 1 calc R U . . . C5 C 0.45644(14) 0.3585(2) 0.41649(11) 0.0277(4) Uani 1 1 d . . . . H5 H 0.5117 0.3929 0.4190 0.033 Uiso 1 1 calc R U . . . C6 C 0.44029(12) 0.2922(2) 0.47732(10) 0.0208(4) Uani 1 1 d . . . . H6 H 0.4848 0.2809 0.5208 0.025 Uiso 1 1 calc R U . . . C11 C 0.43391(11) 0.15548(19) 0.62279(9) 0.0142(3) Uani 1 1 d . . . . C12 C 0.45370(12) 0.2774(2) 0.67061(10) 0.0211(4) Uani 1 1 d . . . . H12 H 0.4144 0.3573 0.6668 0.025 Uiso 1 1 calc R U . . . C13 C 0.53077(13) 0.2825(2) 0.72391(11) 0.0254(4) Uani 1 1 d . . . . H13 H 0.5445 0.3670 0.7555 0.030 Uiso 1 1 calc R U . . . C14 C 0.58765(12) 0.1641(2) 0.73100(10) 0.0243(4) Uani 1 1 d . . . . H14 H 0.6401 0.1674 0.7676 0.029 Uiso 1 1 calc R U . . . C15 C 0.56790(12) 0.0413(2) 0.68466(10) 0.0226(4) Uani 1 1 d . . . . H15 H 0.6064 -0.0403 0.6900 0.027 Uiso 1 1 calc R U . . C16 C 0.49150(11) 0.0374(2) 0.63010(9) 0.0177(3) Uani 1 1 d . . . H16 H 0.4787 -0.0461 0.5978 0.021 Uiso 1 1 calc R U . . . C21 C 0.31644(10) -0.04252(18) 0.52552(9) 0.0141(3) Uani 1 1 d . . . . C22 C 0.34294(11) -0.0989(2) 0.46750(9) 0.0187(4) Uani 1 1 d . . . . H22 H 0.3703 -0.0333 0.4421 0.022 Uiso 1 1 calc R U . . . C23 C 0.33018(13) -0.2494(2) 0.44610(11) 0.0246(4) Uani 1 1 d . . . . H23 H 0.3481 -0.2852 0.4061 0.029 Uiso 1 1 calc R U . . .

C24 C 0.29132(13) -0.3466(2) 0.48329(11) 0.0275(4) Uani 1 1 d . . . . H24 H 0.2830 -0.4494 0.4692 0.033 Uiso 1 1 calc R U . . C25 C 0.26446(13) -0.2933(2) 0.54128(11) 0.0239(4) Uani 1 1 d . . . . H25 H 0.2381 -0.3602 0.5670 0.029 Uiso 1 1 calc R U . . . C26 C 0.27597(11) -0.14233(19) 0.56200(9) 0.0162(3) Uani 1 1 d . . . . C31 C 0.20515(12) 0.4447(2) 0.70991(10) 0.0223(4) Uani 1 1 d . . . . C32 C 0.19105(16) 0.5359(2) 0.76879(11) 0.0318(5) Uani 1 1 d . . . . H32A H 0.1995 0.6426 0.7595 0.048 Uiso 1 1 calc R U . . . H32B H 0.2310 0.5057 0.8149 0.048 Uiso 1 1 calc R U . . . H32C H 0.1332 0.5206 0.7715 0.048 Uiso 1 1 calc R U . . C33 C 0.05033(13) 0.3311(2) 0.46608(11) 0.0264(4) Uani 1 1 d . . . . C34 C -0.03458(14) 0.3589(3) 0.41992(13) 0.0412(6) Uani 1 1 d . . . . H34A H -0.0576 0.2658 0.3944 0.062 Uiso 1 1 calc R U . . . H34B H -0.0329 0.4374 0.3843 0.062 Uiso 1 1 calc R U . . . H34C H -0.0705 0.3923 0.4499 0.062 Uiso 1 1 calc R U . . . N51 N 0.07120(17) 0.2477(3) 0.30431(15) 0.0546(6) Uani 1 1 d . . . . C51 C 0.08544(15) 0.3617(3) 0.28400(13) 0.0384(5) Uani 1 1 d . . . . C52 C 0.1046(2) 0.5061(4) 0.25827(19) 0.0617(9) Uani 1 1 d . . . . H52A H 0.1500 0.5544 0.2958 0.093 Uiso 1 1 calc R U . . . H52B H 0.0542 0.5701 0.2473 0.093 Uiso 1 1 calc R U . . . H52C H 0.1228 0.4922 0.2142 0.093 Uiso 1 1 calc R U . . . N61 N 0.0568(3) 0.6747(4) 0.3922(2) 0.0914(11) Uani 1 1 d . . . . C61 C 0.05593(19) 0.7976(3) 0.40659(14) 0.0464(6) Uani 1 1 d . . . . C62 C 0.05286(19) 0.9540(3) 0.42632(15) 0.0501(7) Uani 1 1 d . . . . H62A H -0.0051 0.9809 0.4251 0.075 Uiso 1 1 calc R U . . . H62B H 0.0715 1.0173 0.3918 0.075 Uiso 1 1 calc R U . . . H62C H 0.0901 0.9701 0.4754 0.075 Uiso 1 1 calc R U . . . loop atom site aniso label \_atom\_site\_aniso U 11 atom site aniso U 22 atom site aniso U 33 atom site aniso U 23 \_atom\_site aniso U 13 atom site aniso U 12 Cu1 0.01443(12) 0.02111(12) 0.01995(12) -0.00067(8) 0.00421(8) 0.00510(8) P1 0.0110(2) 0.0127(2) 0.01380(19) -0.00135(15) 0.00216(15) 0.00074(15) S1 0.0140(2) 0.0191(2) 0.0171(2) 0.00186(16) 0.00407(15) -0.00119(16) 01 0.0182(6) 0.0282(7) 0.0173(6) -0.0012(5) 0.0008(5) -0.0018(5) 02 0.0297(8) 0.0250(7) 0.0302(7) 0.0045(6) 0.0134(6) -0.0057(6) 03 0.0133(6) 0.0278(7) 0.0235(6) 0.0024(5) 0.0049(5) 0.0039(5) N1 0.0220(8) 0.0264(8) 0.0239(8) -0.0015(7) 0.0049(7) 0.0047(7) N2 0.0240(9) 0.0318(9) 0.0252(8) -0.0010(7) 0.0018(7) 0.0087(7) C1 0.0180(8) 0.0118(7) 0.0156(8) -0.0007(6) 0.0049(7) 0.0016(6)  $\texttt{C2} \ \texttt{0.0189(9)} \ \texttt{0.0183(8)} \ \texttt{0.0195(9)} \ \texttt{-0.0019(7)} \ \texttt{0.0014(7)} \ \texttt{0.0018(7)}$ C3 0.0309(11) 0.0209(9) 0.0173(8) 0.0007(7) 0.0013(7) 0.0046(8) C4 0.0380(12) 0.0230(10) 0.0216(9) 0.0056(7) 0.0116(8) 0.0005(8) C5 0.0269(10) 0.0298(10) 0.0276(10) 0.0051(8) 0.0096(8) -0.0051(8)C6 0.0192(9) 0.0231(9) 0.0191(9) 0.0035(7) 0.0035(7) -0.0010(7) C11 0.0140(8) 0.0164(8) 0.0124(7) 0.0009(6) 0.0037(6) -0.0016(6) C12 0.0182(9) 0.0218(9) 0.0220(9) -0.0051(7) 0.0035(7) -0.0005(7) C13 0.0212(10) 0.0306(10) 0.0224(9) -0.0111(8) 0.0030(8) -0.0065(8)C14 0.0142(9) 0.0370(11) 0.0187(9) -0.0010(8) -0.0003(7) -0.0038(8) C15 0.0148(9) 0.0262(10) 0.0248(9) 0.0022(8) 0.0025(7) 0.0027(7) C16 0.0151(8) 0.0195(8) 0.0181(8) -0.0013(7) 0.0037(7) 0.0001(7)  $C21 \ 0.0111(8) \ 0.0138(8) \ 0.0151(8) \ -0.0021(6) \ -0.0002(6) \ 0.0009(6)$ C22 0.0160(8) 0.0202(9) 0.0191(8) -0.0021(7) 0.0036(7) 0.0017(7)

C23 0.0254(10) 0.0232(9) 0.0243(9) -0.0091(7) 0.0056(8) 0.0046(8) C24 0.0297(11) 0.0156(9) 0.0344(11) -0.0070(8) 0.0042(8) 0.0008(8) c25 0.0234(10) 0.0157(8) 0.0312(10) 0.0004(7) 0.0053(8) -0.0020(7) C26 0.0123(8) 0.0171(8) 0.0171(8) -0.0014(6) 0.0006(6) 0.0010(6) C31 0.0234(10) 0.0212(9) 0.0224(9) 0.0034(7) 0.0064(7) 0.0022(7) C32 0.0495(14) 0.0276(10) 0.0235(10) 0.0003(8) 0.0190(9) 0.0038(10) C33 0.0220(10) 0.0284(10) 0.0260(10) -0.0039(8) 0.0023(8) 0.0059(8) C34 0.0211(11) 0.0559(15) 0.0389(12) -0.0071(11) -0.0043(9) 0.0104(10) N51 0.0484(15) 0.0533(15) 0.0623(16) 0.0004(12) 0.0158(12) -0.0082(11) C51 0.0282(12) 0.0565(16) 0.0315(11) 0.0039(11) 0.0101(9) 0.0082(11) c52 0.0564(18) 0.0630(19) 0.079(2) 0.0370(17) 0.0412(17) 0.0240(15) N61 0.126(3) 0.0564(19) 0.094(2) -0.0071(17) 0.033(2) -0.002(2) C61 0.0500(16) 0.0504(16) 0.0368(13) 0.0051(12) 0.0088(11) -0.0002(13) C62 0.0562(17) 0.0496(16) 0.0432(14) 0.0029(12) 0.0118(13) 0.0006(13) #\_\_\_\_\_\_ ---# # MOLECULAR GEOMETRY # #\_\_\_\_\_ ---# \_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 \_geom\_bond\_atom\_site\_label\_2 \_geom\_bond\_distance \_geom\_bond\_site\_symmetry 2 geom bond publ flag Cul N1 1.9931(17) . ? Cul N2 1.9963(17) . ? Cul P1 2.2063(5) . ? Cu1 03 2.2525(14) . ? P1 C11 1.8203(17) . ? P1 C1 1.8316(18) . ? P1 C21 1.8450(17) . ? S1 01 1.4442(13) . ? S1 02 1.4506(14) . ? S1 O3 1.4753(13) . ? S1 C26 1.7905(18) . ? N1 C31 1.136(2) . ? N2 C33 1.135(3) . ? C1 C6 1.390(3) . ? C1 C2 1.402(2) . ? C2 C3 1.389(3) . ? C2 H2 0.9500 . ?

C3 C4 1.391(3) . ?
СЗ НЗ 0.9500 . ?
C4 C5 1.382(3) . ?
С4 Н4 0.9500 . ?
C5 C6 1.396(3) . ?
С5 Н5 0.9500 . ?
С6 Н6 0.9500 . ?
C11 C16 1.395(2) . ?
C11 C12 1.395(2) . ?
C12 C13 1.392(3) . ?
C12 H12 0.9500 . ?
C13 C14 1.389(3) . ?
C13 H13 0.9500 . ?
C14 C15 1.385(3) . ?
C14 H14 0.9500 . ?
C15 C16 1.395(2) . ?
C15 H15 0.9500 . ?
C16 H16 0.9500 . ?
C21 C22 1.396(2) . ?
C21 C26 1.407(2) . ?
C22 C23 1.395(3) . ?
C22 H22 0.9500 . ?
C23 C24 1.385(3) . ?
C23 H23 0.9500 . ?
C24 C25 1.389(3) . ?
C24 H24 0.9500 . ?
C25 C26 1.394(3) . ?
C25 H25 0.9500 . ?
C31 C32 1.458(3) . ?
C32 H32A 0.9800 . ?
C32 H32B 0.9800 . ?
C32 H32C 0.9800 . ?
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C34 H34A 0.9800 . ?
C34 H34B 0.9800 . ?
C34 H34C 0.9800 . ?
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С52 Н52В 0.9800 . ?
C52 H52C 0.9800 . ?
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C61 C62 1.442(4) . ?
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С62 Н62В 0.9800 . ?
C62 H62C 0.9800 . ?
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loop
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N1 Cu1 O3 102.65(6) . . ? N2 Cu1 O3 93.98(6) . . ? P1 Cu1 O3 96.93(4) . . ? C11 P1 C1 103.31(8) . . ? C11 P1 C21 103.57(8) . . ? C1 P1 C21 102.61(8) . . ? C11 P1 Cu1 119.06(6) . . ? C1 P1 Cu1 116.16(6) . . ? C21 P1 Cu1 110.22(6) . . ? O1 S1 O2 114.58(8) . . ? O1 S1 O3 112.30(8) . . ? O2 S1 O3 111.85(8) . . ? O1 S1 C26 106.34(8) . . ? O2 S1 C26 105.97(9) . . ? O3 S1 C26 104.94(8) . . ? S1 O3 Cu1 110.61(7) . . ? C31 N1 Cu1 174.19(16) . . ? C33 N2 Cu1 170.46(19) . . ? C6 C1 C2 118.93(16) . . ? C6 C1 P1 123.01(14) . . ? C2 C1 P1 118.03(14) . . ? C3 C2 C1 120.15(18) . . ? C3 C2 H2 119.9 . . ? C1 C2 H2 119.9 . . ? C2 C3 C4 120.52(18) . . ? C2 C3 H3 119.7 . . ? C4 C3 H3 119.7 . . ? C5 C4 C3 119.57(18) . . ? C5 C4 H4 120.2 . . ? C3 C4 H4 120.2 . . ? C4 C5 C6 120.26(19) . . ? C4 C5 H5 119.9 . . ? C6 C5 H5 119.9 . . ? C1 C6 C5 120.54(18) . . ? C1 C6 H6 119.7 . . ? С5 С6 Н6 119.7 . . ? C16 C11 C12 119.19(16) . . ? C16 C11 P1 122.40(13) . . ? C12 C11 P1 118.41(13) . . ? C13 C12 C11 120.34(18) . . ? C13 C12 H12 119.8 . . ? C11 C12 H12 119.8 . . ? C14 C13 C12 120.09(18) . . ? C14 C13 H13 120.0 . . ? C12 C13 H13 120.0 . . ? . ? C15 C14 C13 119.98(17) . C15 C14 H14 120.0 . . ? C13 C14 H14 120.0 . . ? C14 C15 C16 120.08(18) . . ? C14 C15 H15 120.0 . . ? C16 C15 H15 120.0 . . ? C11 C16 C15 120.30(17) . . ? C11 C16 H16 119.9 . . ? C15 C16 H16 119.9 . . ? C22 C21 C26 117.96(16) . . ? C22 C21 P1 120.77(13) . . ? C26 C21 P1 121.27(13) . . ? C23 C22 C21 121.42(17) . . ?

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C31 C32 H32B 109.5 . . ?
H32A C32 H32B 109.5 . . ?
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H32A C32 H32C 109.5 . . ?
H32B C32 H32C 109.5 . . ?
N2 C33 C34 178.3(2) . . ?
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C33 C34 H34B 109.5 . . ?
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H34B C34 H34C 109.5 . . ?
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N61 C61 C62 178.1(4) . .
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02 S1 O3 Cu1 169.81(7) . . . ?
C26 S1 O3 Cu1 -75.75(9) . . . ?
C11 P1 C1 C6 -1.25(17) . . . ?
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C21 P1 C1 C6 -108.71(15) . . . ? Cul Pl Cl C6 130.99(14) . . . ? C11 P1 C1 C2 -179.45(13) . . . ? C21 P1 C1 C2 73.09(14) . . . ? Cul Pl Cl C2 -47.21(15) . . . ? C6 C1 C2 C3 1.9(3) . . . ? P1 C1 C2 C3 -179.83(14) . . . ? C1 C2 C3 C4 - 1.5(3) . . . ?C2 C3 C4 C5 0.0(3) . . . ? C3 C4 C5 C6 1.1(3) . . . ? C2 C1 C6 C5 -0.9(3) . . . ? P1 C1 C6 C5 -179.05(15) . . . ? C4 C5 C6 C1 -0.6(3) . . . ? C1 P1 C11 C16 -87.09(15) . . . ? C21 P1 C11 C16 19.65(16) . . . ? Cul P1 C11 C16 142.39(13) . . . ? C1 P1 C11 C12 92.72(15) . . . ? C21 P1 C11 C12 -160.54(14) . . . ? Cu1 P1 C11 C12 -37.80(16) . . . ? C16 C11 C12 C13 1.4(3) . . . ? P1 C11 C12 C13 -178.42(15) . . . ? C11 C12 C13 C14 -1.7(3) . . . ? C12 C13 C14 C15 0.4(3) . . . ? C13 C14 C15 C16 1.0(3) . . . ? C12 C11 C16 C15 0.1(3) . . . ? P1 C11 C16 C15 179.87(14) . . . ? C14 C15 C16 C11 -1.3(3) . . . ? C11 P1 C21 C22 -92.77(15) . . . ? C1 P1 C21 C22 14.49(16) . . . ? Cul P1 C21 C22 138.81(13) . . . ? C11 P1 C21 C26 87.78(15) . . . ? C1 P1 C21 C26 -164.96(14) . . . ? Cu1 P1 C21 C26 -40.63(15) . . . ? C26 C21 C22 C23 - 0.2(3) . . . ?P1 C21 C22 C23 -179.64(14) . . . ? C21 C22 C23 C24 -0.7(3) . . . . ? C22 C23 C24 C25 0.6(3) . . . ? C23 C24 C25 C26 0.4(3) . . . ? C24 C25 C26 C21 -1.3(3) . . . ? C24 C25 C26 S1 178.13(15) . . . ? C22 C21 C26 C25 1.2(3) . . . ? P1 C21 C26 C25 -179.34(14) . . . ? C22 C21 C26 S1 -178.22(13) . . . P1 C21 C26 S1 1.2(2) . . . ? 01 S1 C26 C25 127.16(15) . . . ? O2 S1 C26 C25 4.84(17) . . . ? O3 S1 C26 C25 -113.66(15) . . . ? O1 S1 C26 C21 -53.40(16) . . . ? 02 S1 C26 C21 -175.73(14) . . . ? O3 S1 C26 C21 65.78(16) . . . ? #\_\_\_\_\_ ---# #===END OF CIF FILE FOR MACU1ACN # #\_\_\_\_\_\_ ----# \*\*\*\*\*\*

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# This file contains crystal structure data downloaded from the
# Cambridge Structural Database (CSD) hosted by the Cambridge
# Crystallographic Data Centre (CCDC).
#
# Full information about CCDC data access policies and citation
# guidelines are available at http://www.ccdc.cam.ac.uk/access/V1
#
# Audit and citation data items may have been added by the CCDC.
# Please retain this information to preserve the provenance of
# this file and to allow appropriate attribution of the data.
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'-x, -y, -z'
cell length a
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\_cell\_length\_b 9.9958(7) \_cell\_length\_c 12.8416(10) \_cell\_angle\_alpha 109.783(2)\_cell\_angle\_beta 108.389(2) \_cell\_angle\_gamma 93.792(2) \_cell\_volume 943.65(13) cell formula units Z 1 \_cell\_measurement\_temperature 150(2) \_cell\_measurement\_reflns\_used 9938 \_cell\_measurement\_theta\_min2.26\_cell\_measurement\_theta\_max27.50\_cell\_measurement\_wavelength0.71073 #\_\_\_\_\_ ---# # CRYSTAL INFORMATION # #--------# \_exptl\_crystal\_description prism exptl\_crystal\_colour colourless 0.470 0.410 \_exptl\_crystal\_size max exptl crystal size mid \_exptl\_crystal\_size\_min 0.120 \_exptl\_crystal\_density\_meas
\_exptl\_crystal\_density\_diffrn 1.499
\_\_\_\_\_\_density\_method ? exptl crystal F 000 440 \_exptl\_special\_details ; ? ; #\_\_\_\_\_ ---# # ABSORPTION CORRECTION # ---# exptl absorpt coefficient mu 1.369 \_exptl\_absorpt\_correction\_type multi-scan \_exptl\_absorpt\_process\_details ; [Sheldrick, G.M. (2014). SADABS Bruker AXS Inc., Madison, Wisconsin, USA] ; \_exptl\_absorpt\_correction T min 0.727 exptl absorpt correction T max 0.849 #\_\_\_\_\_ ---# # DATA COLLECTION # #\_\_\_\_\_\_ ---#

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                      COMPUTER PROGRAMS USED
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_computing_structure_solution 'SIR97 (Altomare et al., 1999)'
_computing_structure_refinement 'SHELXL-2014/7 (Sheldrick, 2014)'
computing molecular graphics 'Ortep-3 for Windows (Farrugia, 1997)'
computing publication material 'CRYSCALc (T. Roisnel, local program,
2015)'
#______
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#
                     REFINEMENT INFORMATION
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#_____
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_refine_special details
Refinement of F^2^ against ALL reflections. The weighted R-factor wR and
```

goodness of fit S are based on  $F^{2^{\circ}}$ , conventional R-factors R are based on F, with F set to zero for negative  $F^{2^{\circ}}$ . The threshold expression of  $F^{2^{\circ}} > 2 \text{sigma}(F^{2^{\circ}})$  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 Rfactors based on ALL data will be even larger. \_refine\_ls\_structure factor coef Fsqd refine ls matrix type full refine ls weighting scheme calc refine ls weighting details  $w=1/[\sqrt{s^2}(Fo^2)+(0.0412P)^2+0.5991P]$  where  $P=(Fo^2+2Fc^2)/3'$ \_atom\_sites\_solution\_primary ? \_atom\_sites\_solution secondary ? atom sites solution hydrogens geom \_refine\_ls\_hydrogen\_treatment constr \_refine\_ls\_extinction method none \_refine\_ls\_extinction\_coef \_refine\_ls\_number\_reflns 4317 \_refine\_ls\_number\_parameters 230 \_refine\_ls\_number restraints 0 \_refine\_ls\_R\_factor\_all 0.0295 \_refine\_ls\_R\_factor\_gt 0.0280 \_refine\_ls\_wR\_factor ref 0.0826 \_refine\_ls\_wR\_factor gt 0.0813 refine ls goodness of fit ref 1.180 1.180 refine ls restrained S all \_refine\_ls\_shift/su max 0.001 \_refine\_ls\_shift/su\_mean 0.000 refine diff density max 0.617 \_refine\_diff\_density min -0.753 refine diff density rms 0.175 \_iucr\_refine\_instructions\_details .res SHELXL file: MACuO6.res MACuO6.res created by SHELXL-2014/7 TITL import a.res in P-1 CELL 0.71073 8.3918 9.9958 12.8416 109.783 108.389 93.792 ZERR 1.00 0.0007 0.0007 0.0010 0.002 0.002 0.002 1 LATT SFAC C Н Ρ S CU Ν 0 2 2 2 2 UNIT 36 42 6 MERG 2 2 FMAP PLAN 20 0.12 0.41 0.47 SIZE ACTA BOND \$Н CONF 4 LIST WPDB -2 L.S. 4 TEMP -123.00 WGHT 0.041200 0.599100 0.78736 FVAR

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AFIX 0 1 0.499451 0.684171 0.270496 11.00000 0.02260 C8 0.01403 =0.01464 0.00491 0.00750 0.00675 1 0.284544 0.766852 0.089948 11.00000 0.01929 С9 0.01889 =0.01240 0.00349 0.00567 0.00090 c10 1 0.237561 0.618749 0.020458 11.00000 0.03100 0.02088 =0.01999 0.00071 0.00909 -0.00069 AFIX 43 0.304261 0.553926 0.044465 11.00000 -1.20000 H10 2 0 AFIX 1 0.094769 0.565321 -0.083092 11.00000 0.03272 C11 0.03489 =0.01993 -0.00409 0.00749 -0.00950 AFIX 43 2 0.062694 0.464135 -0.128822 11.00000 -1.20000 Н11 AFIX 0 1 -0.000978 C12 0.659073 -0.119879 11.00000 0.02394 0.05867 =0.01896 0.00546 -0.00112 -0.00690 AFIX 43 H12 2 -0.098307 0.622468 -0.191275 11.00000 -1.20000 0 AFIX c13 1 0.044757 0.806095 -0.052867 11.00000 0.03162 0.05446 =0.03266 0.01604 -0.00544 0.01110 AFIX 43 H13 2 -0.020366 0.870557 -0.078876 11.00000 -1.20000 AFIX 0 C14 1 0.186104 0.860204 0.052772 11.00000 0.02820 0.02827 =0.02635 0.00787 -0.00281 0.00574 AFIX 43 0.961116 0.099520 11.00000 -1.20000 2 0.215306 H14 0 AFIX C15 1 0.650720 0.901644 0.193205 11.00000 0.02153 0.01766 =0.02543 0.00623 0.01309 0.00306 c16 1 0.623316 1.048479 0.183036 11.00000 0.03803 0.02055 =0.05013 0.01622 0.02518 0.00451 AFIX 137 H16A 2 0.715079 11.00000 -1.50000 1.086415 0.162691 
 11.00000
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 11.00000
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0.03855 0.00771 0.00859 0.00396 AFIX 137 H18A20.8379060.8359630.30522311.00000-1.50000H18B20.8051980.9928380.37164711.00000-1.50000H18C20.9123500.9736750.28594011.00000-1.50000 AFIX 0 HKLF 4 REM import a.res in P-1 REM R1 = 0.0280 for 4128 Fo > 4sig(Fo) and 0.0295 for all 4317 data 230 parameters refined using 0 restraints REM END WGHT 0.0412 0.5991 REM Highest difference peak 0.617, deepest hole -0.753, 1-sigma level 0.175 1 0.3588 0.8030 0.1917 11.00000 0.05 Q1 0.62 1 0.2221 0.8043 0.0830 11.00000 0.05 0.48 Q2 1 0.9096 0.9348 0.2810 11.00000 0.05 0.45 Q3 1 0.6799 1.0200 0.6569 11.00000 0.05 0.45 Q4 1 0.2669 0.6953 0.0584 11.00000 0.05 0.43 Q5 1 0.8306 0.8532 0.3459 11.00000 0.05 0.43 06 1 0.8811 0.6933 0.3128 11.00000 0.05 0.42 Q7 1 0.0273 0.3646 -0.2566 11.00000 0.05 0.41 Q8 1 0.8469 0.6463 0.3514 11.00000 0.05 0.41 Q9 1 0.9199 1.0840 0.2977 11.00000 0.05 0.40 Q10 1 0.1677 0.9690 0.1377 11.00000 0.05 0.40 Q11 Q12 1 0.9937 1.1299 0.2840 11.00000 0.05 0.40 Q13 1 -0.1297 0.5218 -0.1854 11.00000 0.05 0.39 014 1 0.0706 0.7121 0.3189 11.00000 0.05 0.39 Q15 1 -0.1298 0.4838 -0.2021 11.00000 0.05 0.39 Q16 1 1.0245 1.0624 0.2414 11.00000 0.05 0.39 Q1011.02431.00240.241411.000000.050.39Q1710.79810.63430.379711.000000.050.39Q181-0.02240.74480.264011.000000.050.37Q1910.09540.97730.208411.000000.050.37Q2010.90380.60060.292111.000000.050.37 ; shelx res checksum 38569 # End of res file # .hkl SHELXL file: MACuO6.hkl # ---# #\_\_\_\_\_\_ ---# # ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS # #\_\_\_\_\_ ---#

loop\_ \_atom\_type\_symbol \_atom\_type\_description atom type scat dispersion real \_atom\_type\_scat\_dispersion imag atom type scat source C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' P P 0.1023 0.0942 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' S S 0.1246 0.1234 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' Cu Cu 0.3201 1.2651 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' N N 0.0061 0.0033 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' 0 0 0.0106 0.0060 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4' loop atom site label atom site type symbol \_atom\_site\_fract\_x \_atom\_site\_fract\_y atom site fract z atom site U iso or equiv \_atom\_site\_adp\_type atom site occupancy atom site site symmetry order \_atom\_site\_calc flag \_atom\_site\_refinement flags posn atom site refinement flags adp \_atom\_site\_refinement\_flags\_occupancy \_atom\_site\_disorder assembly atom site disorder group Cul Cu 0.57981(3) 0.98171(2) 0.63035(2) 0.01697(8) Uani 1 1 d . . . . P1 P 0.46502(5) 0.84312(4) 0.23058(4) 0.01329(10) Uani 1 1 d . . . . N1 N 0.7236(2) 0.83816(17) 0.61387(14) 0.0214(3) Uani 1 1 d . . . S1 S 0.26279(5) 0.74253(4) 0.38804(4) 0.01622(10) Uani 1 1 d . . . 01 0 0.35877(16) 0.89052(13) 0.46903(11) 0.0169(2) Uani 1 1 d . . . . 02 0 0.2038(2) 0.66666(16) 0.45107(15) 0.0314(3) Uani 1 1 d . . . . O3 O 0.13432(17) 0.74479(15) 0.28308(13) 0.0260(3) Uani 1 1 d . . . . C1 C 0.8185(2) 0.76437(19) 0.59901(17) 0.0209(4) Uani 1 1 d . . . . C2 C 0.9410(3) 0.6710(2) 0.5806(2) 0.0337(5) Uani 1 1 d . . . . H2A H 0.9703 0.6735 0.5131 0.051 Uiso 1 1 calc R U . . . H2B H 0.8906 0.5714 0.5643 0.051 Uiso 1 1 calc R U . . H2C H 1.0447 0.7051 0.6520 0.051 Uiso 1 1 calc R U . . . C3 C 0.4138(2) 0.64533(18) 0.33777(15) 0.0152(3) Uani 1 1 d . . . . C4 C 0.4391(2) 0.52375(19) 0.36569(16) 0.0206(4) Uani 1 1 d . . . . H4 H 0.3808 0.4997 0.4114 0.025 Uiso 1 1 calc R U . . . C5 C 0.5481(3) 0.4368(2) 0.32779(19) 0.0280(4) Uani 1 1 d . . . . H5 H 0.5637 0.3534 0.3468 0.034 Uiso 1 1 calc R U . . . C6 C 0.6333(3) 0.4730(2) 0.2624(2) 0.0326(5) Uani 1 1 d . . . . H6 H 0.7085 0.4145 0.2362 0.039 Uiso 1 1 calc R U . C7 C 0.6094(3) 0.5950(2) 0.23452(19) 0.0275(4) Uani 1 1 d . . . . H7 H 0.6697 0.6186 0.1897 0.033 Uiso 1 1 calc R U . . . C8 C 0.4995(2) 0.68417(18) 0.27050(15) 0.0169(3) Uani 1 1 d . . . . C9 C 0.2845(2) 0.76685(19) 0.08995(15) 0.0177(3) Uani 1 1 d . . . . C10 C 0.2376(3) 0.6187(2) 0.02046(17) 0.0262(4) Uani 1 1 d . . . . H10 H 0.3043 0.5539 0.0445 0.031 Uiso 1 1 calc R U . . . C11 C 0.0948(3) 0.5653(3) -0.08309(18) 0.0345(5) Uani 1 1 d . . . .

H11 H 0.0627 0.4641 -0.1288 0.041 Uiso 1 1 calc R U . . C12 C -0.0010(3) 0.6591(3) -0.11988(19) 0.0395(6) Uani 1 1 d . . . . H12 H -0.0983 0.6225 -0.1913 0.047 Uiso 1 1 calc R U . . C13 C 0.0448(3) 0.8061(3) -0.0529(2) 0.0440(6) Uani 1 1 d . . . . H13 H -0.0204 0.8706 -0.0789 0.053 Uiso 1 1 calc R U . . . C14 C 0.1861(3) 0.8602(2) 0.05277(19) 0.0315(5) Uani 1 1 d . . . . H14 H 0.2153 0.9611 0.0995 0.038 Uiso 1 1 calc R U . . . C15 C 0.6507(2) 0.9016(2) 0.19320(17) 0.0209(4) Uani 1 1 d . . . . C16 C 0.6233(3) 1.0485(2) 0.1830(2) 0.0331(5) Uani 1 1 d . . . . H16A H 0.7151 1.0864 0.1627 0.050 Uiso 1 1 calc R U . . . H16B H 0.6248 1.1172 0.2590 0.050 Uiso 1 1 calc R U . . . H16C H 0.5126 1.0351 0.1210 0.050 Uiso 1 1 calc R U . . . C17 C 0.6597(3) 0.8017(2) 0.0752(2) 0.0321(5) Uani 1 1 d . . . . . H17A H 0.7514 0.8473 0.0591 0.048 Uiso 1 1 calc R U . . . H17B H 0.5502 0.7851 0.0111 0.048 Uiso 1 1 calc R U . . . H17C H 0.6833 0.7089 0.0802 0.048 Uiso 1 1 calc R U . . . C18 C 0.8165(3) 0.9285(3) 0.2985(2) 0.0349(5) Uani 1 1 d . . . . . H18A H 0.8379 0.8360 0.3052 0.052 Uiso 1 1 calc R U . . . H18B H 0.8052 0.9928 0.3716 0.052 Uiso 1 1 calc R U . . H18C H 0.9123 0.9737 0.2859 0.052 Uiso 1 1 calc R U . . . loop atom site aniso label atom site aniso U 11 atom site aniso U 22 atom site aniso U 33 atom site aniso U 23 \_atom\_site aniso U 13 atom site aniso U 12 Cu1 0.02345(13) 0.01257(12) 0.01443(12) 0.00303(8) 0.00797(9) 0.00610(8) P1 0.0166(2) 0.0113(2) 0.01126(19) 0.00310(15) 0.00507(15) 0.00387(15) N1 0.0242(8) 0.0162(7) 0.0226(8) 0.0055(6) 0.0084(6) 0.0053(6) s1 0.01578(19) 0.0118(2) 0.0192(2) 0.00277(16) 0.00756(16) 0.00091(14) 01 0.0201(6) 0.0130(6) 0.0138(6) 0.0009(5) 0.0063(5) 0.0005(4) 02 0.0395(8) 0.0220(7) 0.0483(9) 0.0165(7) 0.0321(8) 0.0076(6) 03 0.0170(6) 0.0236(7) 0.0249(7) 0.0006(6) 0.0008(5) 0.0037(5) C1 0.0209(8) 0.0147(8) 0.0263(9) 0.0065(7) 0.0094(7) 0.0014(7) C2 0.0265(10) 0.0228(10) 0.0599(15) 0.0158(10) 0.0249(10) 0.0106(8) C3 0.0172(8) 0.0125(8) 0.0130(7) 0.0026(6) 0.0039(6) 0.0029(6) C4 0.0268(9) 0.0168(9) 0.0184(8) 0.0075(7) 0.0078(7) 0.0041(7) C5 0.0426(12) 0.0202(9) 0.0292(10) 0.0147(8) 0.0158(9) 0.0158(8) C6 0.0479(13) 0.0305(11) 0.0369(11) 0.0196(9) 0.0266(10) 0.0274(10) C7 0.0400(11) 0.0269(10) 0.0308(10) 0.0164(8) 0.0240(9) 0.0200(9) C8 0.0226(8) 0.0140(8) 0.0146(8) 0.0049(6) 0.0075(7) 0.0067(6) C9 0.0193(8) 0.0189(9) 0.0124(7) 0.0035(6) 0.0057(6) 0.0009(6) c10 0.0310(10) 0.0209(9) 0.0200(9) 0.0007(7) 0.0091(8) -0.0007(7) C11 0.0327(11) 0.0349(12) 0.0199(10) -0.0041(8) 0.0075(9) -0.0095(9) C12 0.0239(10) 0.0587(16) 0.0190(10) 0.0055(10) -0.0011(8) -0.0069(10) C13 0.0316(12) 0.0545(16) 0.0327(12) 0.0160(11) -0.0054(10) 0.0111(11) C14 0.0282(10) 0.0283(11) 0.0263(10) 0.0079(8) -0.0028(8) 0.0057(8) C15 0.0215(8) 0.0177(8) 0.0254(9) 0.0062(7) 0.0131(7) 0.0031(6) C16 0.0380(12) 0.0205(10) 0.0501(13) 0.0162(9) 0.0252(10) 0.0045(8) c17 0.0477(13) 0.0261(10) 0.0334(11) 0.0107(9) 0.0293(10) 0.0084(9) C18 0.0188(9) 0.0398(12) 0.0385(12) 0.0077(10) 0.0086(9) 0.0040(8)

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#
                               MOLECULAR GEOMETRY
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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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Cu1 01 2.1533(12) . ?
Cul P1 2.1889(5) 2 676 ?
Cul Ol 2.2264(12) 2 676 ?
P1 C9 1.8237(18) . ?
P1 C8 1.8410(17) . ?
P1 C15 1.8821(18) . ?
P1 Cu1 2.1889(5) 2 676 ?
N1 C1 1.137(2) . ?
S1 O3 1.4444(14) . ?
S1 02 1.4470(14) . ?
S1 01 1.4803(12) . ?
S1 C3 1.7950(17) . ?
O1 Cu1 2.2264(12) 2 676 ?
C1 C2 1.454(3) . ?
C2 H2A 0.9800 . ?
C2 H2B 0.9800 . ?
C2 H2C 0.9800 . ?
C3 C4 1.390(2) . ?
C3 C8 1.412(2) . ?
C4 C5 1.389(3) . ?
C4 H4 0.9500 . ?
C5 C6 1.378(3) . ?
C5 H5 0.9500 . ?
C6 C7 1.392(3) . ?
C6 H6 0.9500 . ?
C7 C8 1.399(2) . ?
C7 H7 0.9500 . ?
C9 C14 1.391(3) . ?
C9 C10 1.396(3) . ?
C10 C11 1.385(3) . ?
C10 H10 0.9500 . ?
C11 C12 1.381(4) . ?
C11 H11 0.9500 . ?
C12 C13 1.381(4) . ?
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C12 H12 0.9500 . ? C13 C14 1.394(3) . ? C13 H13 0.9500 . ? C14 H14 0.9500 . ? C15 C18 1.535(3) . ? C15 C17 1.535(3) . ? C15 C16 1.543(3) . ? C16 H16A 0.9800 . ? C16 H16B 0.9800 . ? C16 H16C 0.9800 . ? C17 H17A 0.9800 . ? C17 H17B 0.9800 . ? C17 H17C 0.9800 . ? C18 H18A 0.9800 . ? C18 H18B 0.9800 . ? C18 H18C 0.9800 . ? loop \_geom\_angle\_atom\_site label 1 \_geom\_angle\_atom\_site\_label\_ 2 \_geom\_angle\_atom\_site\_label\_3 geom angle \_geom\_angle\_site\_symmetry 1 \_geom\_angle\_site\_symmetry 3 geom angle publ flag N1 Cu1 O1 103.91(6) . . ? N1 Cu1 P1 139.73(5) . 2 676 ? O1 Cu1 P1 112.82(4) . 2 676 ? N1 Cu1 O1 103.44(6) . 2 676 ? O1 Cu1 O1 80.36(5) . 2 676 ? P1 Cu1 O1 98.52(3) 2 676 2 676 ? C9 P1 C8 102.49(8) . . ? C9 P1 C15 105.38(8) . . ? C8 P1 C15 109.22(8) . . ? C9 P1 Cu1 114.63(6) . 2\_676 ? C8 P1 Cu1 111.75(6) . 2 676 ? C15 P1 Cu1 112.69(6) . 2\_676 ? C1 N1 Cu1 171.22(16) . . O3 S1 O2 115.97(10) . . ? O3 S1 O1 111.09(8) . . ? 02 S1 01 111.10(9) . . ? O3 S1 C3 105.86(8) . . ? O2 S1 C3 105.75(8) . . ? O1 S1 C3 106.32(8) . . ? S1 O1 Cu1 135.52(8) . . ? S1 O1 Cu1 111.41(7) . 2\_676 ? Cul Ol Cul 99.64(5) . 2 676 ? N1 C1 C2 179.5(2) . . ? C1 C2 H2A 109.5 . . ? C1 C2 H2B 109.5 . . ? H2A C2 H2B 109.5 . . ? C1 C2 H2C 109.5 . . ? H2A C2 H2C 109.5 . . ? H2B C2 H2C 109.5 . . ? C4 C3 C8 120.73(16) . . ? C4 C3 S1 115.79(13) . . ? C8 C3 S1 123.44(13) . . ? C5 C4 C3 121.05(17) . . ?

C5 C4 H4 119.5 . . ? C3 C4 H4 119.5 . . ? C6 C5 C4 119.16(18) . . ? C6 C5 H5 120.4 . . ? C4 C5 H5 120.4 . . ? C5 C6 C7 120.15(18) . . ? C5 C6 H6 119.9 . . ? С7 С6 Н6 119.9 . . ? C6 C7 C8 122.10(18) . . ? C6 C7 H7 118.9 . . ? C8 C7 H7 118.9 . . ? C7 C8 C3 116.80(16) . . ? C7 C8 P1 121.83(14) . . ? C3 C8 P1 121.36(13) . . ? C14 C9 C10 118.79(18) . . ? C14 C9 P1 118.28(14) . . ? C10 C9 P1 122.89(15) . . ? C11 C10 C9 120.7(2) . . ? C11 C10 H10 119.6 . . ? C9 C10 H10 119.6 . . ? C12 C11 C10 120.0(2) . . ? C12 C11 H11 120.0 . . ? C10 C11 H11 120.0 . . ? C11 C12 C13 120.0(2) . . ? C11 C12 H12 120.0 . . ? C13 C12 H12 120.0 . . ? C12 C13 C14 120.2(2) . . ? C12 C13 H13 119.9 . . ? C14 C13 H13 119.9 . . ? C9 C14 C13 120.2(2) . . ? C9 C14 H14 119.9 . . ? C13 C14 H14 119.9 . . ? C18 C15 C17 112.29(17) . . ? C18 C15 C16 108.19(18) . . ? C17 C15 C16 107.35(17) . . ? C18 C15 P1 108.49(14) . . ? C17 C15 P1 115.73(14) . . ? C16 C15 P1 104.24(13) . . ? C15 C16 H16A 109.5 . . ? C15 C16 H16B 109.5 . . ? H16A C16 H16B 109.5 . . ? C15 C16 H16C 109.5 . . ? H16A C16 H16C 109.5 . . ? H16B C16 H16C 109.5 . . ? C15 C17 H17A 109.5 . . ? C15 C17 H17B 109.5 . . ? H17A C17 H17B 109.5 . . ? C15 C17 H17C 109.5 . . ? H17A C17 H17C 109.5 . . ? H17B C17 H17C 109.5 . . ? C15 C18 H18A 109.5 . . ? C15 C18 H18B 109.5 . . ? H18A C18 H18B 109.5 . . ? C15 C18 H18C 109.5 . . ? H18A C18 H18C 109.5 . . ? H18B C18 H18C 109.5 . . ?

loop\_

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02 S1 O1 Cu1 56.55(13) . . .
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O3 S1 O1 Cu1 -41.76(10) . . . 2 676 ?
O2 S1 O1 Cu1 -172.46(8) . . . 2 676 ?
C3 S1 O1 Cu1 72.95(8) . . . 2_676 ?
O3 S1 C3 C4 -122.43(14) . . . ?
O2 S1 C3 C4 1.15(16) . . . ?
O1 S1 C3 C4 119.34(14) . . . ?
O3 S1 C3 C8 55.49(16) . . . ?
O2 S1 C3 C8 179.07(15) . . . ?
O1 S1 C3 C8 -62.74(16) . . . ?
C8 C3 C4 C5 -0.4(3) . . . ?
S1 C3 C4 C5 177.62(15) . . . ?
C3 C4 C5 C6 0.5(3) . . . ?
C4 C5 C6 C7 -0.2(4) . . . ?
C5 C6 C7 C8 -0.3(4) . . . ?
C6 C7 C8 C3 0.5(3) . . . ?
C6 C7 C8 P1 -178.65(18) . . . ?
C4 C3 C8 C7 -0.2(3) . . . ?
S1 C3 C8 C7 -177.98(15) . . . ?
C4 C3 C8 P1 179.00(13) . . . ?
S1 C3 C8 P1 1.2(2) . . . ?
C9 P1 C8 C7 89.85(17) . . . ?
C15 P1 C8 C7 -21.54(19) . . . ?
Cul P1 C8 C7 -146.92(15) 2_676 . . . ?
C9 P1 C8 C3 -89.26(15) . . . ?
C15 P1 C8 C3 159.35(14) . . . ?
Cul P1 C8 C3 33.98(16) 2_676 . . . ?
C8 P1 C9 C14 158.55(16) . . . ?
C15 P1 C9 C14 -87.21(17) . . . ?
Cul P1 C9 C14 37.27(18) 2 676 . . . ?
C8 P1 C9 C10 -19.10(17) . . . ?
C15 P1 C9 C10 95.14(16) . . .
Cul P1 C9 C10 -140.37(14) 2_676 . . . ?
C14 C9 C10 C11 -0.6(3) . . . ?
P1 C9 C10 C11 177.08(16) . . . ?
C9 C10 C11 C12 1.3(3) . . . ?
C10 C11 C12 C13 -0.6(4) . . . ?
C11 C12 C13 C14 -0.9(4) . . . ?
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P1 C9 C14 C13 -178.60(19) . . . ?
C12 C13 C14 C9 1.6(4) . . . ?
C9 P1 C15 C18 -164.83(14) . . . ?
C8 P1 C15 C18 -55.36(15) . . . ?
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C9 P1 C15 C17 -37.58(17) . . . ?
C8 P1 C15 C17 71.89(17) . . . ?
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#_____
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#===END OF CIF FILE FOR MACUO6
#
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*********
#
# This file contains crystal structure data downloaded from the
# Cambridge Structural Database (CSD) hosted by the Cambridge
# Crystallographic Data Centre (CCDC).
# Full information about CCDC data access policies and citation
# guidelines are available at http://www.ccdc.cam.ac.uk/access/V1
#
# Audit and citation data items may have been added by the CCDC.
# Please retain this information to preserve the provenance of
# this file and to allow appropriate attribution of the data.
***************
data MACU88
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2018-07-24 deposited with the CCDC.
2019-01-11 downloaded from the CCDC.
#______
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chemical formula sum
chemical formula weight
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chemical compound source
                       'synthesis as described'
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#
                    UNIT CELL INFORMATION
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\_space\_group\_crystal\_system Monoclinic space group name H-M alt 'P 21/n' \_\_\_\_\_\_space\_group\_name\_H-M\_alt 'P 21/n' '-P 2yn' space group name Hall space group IT number 14 loop space group symop operation xyz 'x, y, z' '-x+1/2, y+1/2, -z+1/2' '-x, -y, -z' 'x-1/2, -y-1/2, z-1/2' cell length a 8.7999(8) \_cell\_length b 18.226(2) cell length c 17.1438(19) 90 cell angle beta 96.313(4) \_cell\_angle\_gamma 90 \_cell\_volume 2733.0(5) \_cell\_formula\_units Z 4 \_cell\_measurement\_temperature150\_cell\_measurement\_reflns\_used9721\_cell\_measurement\_theta\_min2.39\_cell\_measurement\_theta\_max27.46\_cell\_measurement\_wavelength0.71073 #--------# # CRYSTAL INFORMATION # #\_\_\_\_\_ ---# \_exptl\_crystal\_description prism colourless 0.350 0.290 \_exptl\_crystal\_colour \_exptl\_crystal\_size\_max \_exptl\_crystal\_size\_mid \_exptl\_crystal\_size\_min 0.230 \_exptl\_crystal\_density\_meas ? \_exptl\_crystal\_density\_diffrn 1.429 exptl crystal density method ? \_exptl\_crystal F 000 1216 \_exptl\_special\_details ; ? ; #\_\_\_\_\_\_ ---# # ABSORPTION CORRECTION # #\_\_\_\_\_\_ ---# exptl absorpt coefficient mu 0.975 exptl absorpt correction type multi-scan exptl absorpt process details

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[Sheldrick, G.M. (2014). SADABS Bruker AXS Inc., Madison, Wisconsin,
USA]
;
exptl absorpt correction T min 0.670
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2014)'
_computing_data reduction
                                                                    'SAINT (Bruker, 2014)'
_computing_structure_solution 'SHELXT (Sheldrick, 2015)'
_ computing_structure_refinement 'SHELXL-2014/7 (Sheldrick, 2014)'
_ computing_molecular_graphics 'Ortep-3 for Windows (Farrugia, 1997)'
 computing publication material 'CRYSCALc (T. Roisnel, local program,
2015)'
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---# # REFINEMENT INFORMATION # #\_\_\_\_\_\_ ---# \_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  $F^{2^{-1}}$ . 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  $F^{2^{-1}}$  are statistically about twice as large as those based on F, and Rfactors based on ALL data will be even larger. \_refine\_ls\_structure\_factor\_coef Fsqd \_refine\_ls\_matrix\_type full \_refine\_ls\_weighting\_scheme calc refine ls weighting details  $w=1/[s^2(Fo^2)+(0.0341P)^2+2.4761P]$  where  $P=(Fo^2+2Fc^2)/3$ atom sites solution primary ? atom sites solution secondary ? \_atom\_sites\_solution\_hydrogens geom \_refine\_ls\_hydrogen\_treatment constr \_refine\_ls\_extinction\_method none refine ls extinction coef refine ls number reflns 6262 refine ls number parameters 339 refine ls number restraints 0 \_refine\_ls\_R\_factor\_all 0.0354 \_refine\_ls\_R\_factor\_gt 0.0281 \_refine\_ls\_wR\_factor\_ref 0.0769 \_refine\_ls\_wR\_factor\_gt 0.0723 \_refine\_ls\_goodness\_of\_fit\_ref 0.963 \_refine\_ls\_restrained\_S\_all 0.963 refine ls shift/su max 0.004 refine ls shift/su mean 0.000 \_refine\_diff\_density max 0.287 \_refine\_diff\_density\_min -0.491 \_refine\_diff\_density rms 0.059 . . . . . . . # .RES SHELXL file: job.res # .HKL SHELXL file: job.hkl . . . . . . . \_shelx\_res\_file job.res created by SHELXL-2014/7

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 Ν 12 MERG 2 FMAP 2 20 PLAN ACTA \$H BOND CONF LIST 4 WPDB -2 L.S. 4 TEMP -123.00 WGHT 0.034100 2.476100 FVAR 0.43183 MOLE 1 CU1 4 0.770622 0.687596 0.747197 11.00000 0.01896 0.01567 = 0.01387 -0.00114 -0.00303 -0.00367 3 0.674142 0.614277 0.651293 11.00000 0.00920 P1 0.00990 =0.00921 0.00043 -0.00005 -0.00066 7 0.862113 0.657825 0.853559 11.00000 0.03565 N1 0.02042 =0.02073 0.00038 -0.00819 -0.00734 C2 1 0.912671 0.648085 0.916628 11.00000 0.03232 0.02093 =0.02100 -0.00039 -0.00437 -0.00436 C3 1 0.978284 0.635468 0.997530 11.00000 0.05192 0.04224 = 0.01696 0.00411 -0.00779 -0.00184 AFIX 137 1.0826580.6166220.99788011.00000-1.500000.9158130.5995851.02222711.00000-1.500000.9804020.6817331.02675811.00000-1.50000 H3A 2 1.082658 нзв 2 HЗC 2 AFIX O 11.00000 7 0.881659 0.779116 0.723423 N4 0.02234 0.01898 = 0.01928 -0.00172 -0.00108 -0.00337 C5 0.956245 0.827322 0.708308 11.00000 0.02171 1 0.01673 =0.02054 -0.00318 0.00011 0.00015 C6 1 1.052259 0.888208 0.688947 11.00000 0.03152 0.01790 =0.04433 0.00021 0.00742 -0.00614 AFIX 137 1.160078 0.874396 0.700151 11.00000 -1.50000 H6A 2 0.931108 0.720532 0.633117 2 -1.50000 H6B 1.031335 0.900128 -1.50000 H6C 2 1.030033 AFIX 0 0.01535 C11 1 0.655613 0.649468 0.550685 11.00000 0.00959 =0.01027 -0.00021 0.00101 0.00266

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C3 C 0.9783(3) 0.63547(13) 0.99753(12) 0.0379(5) Uani 1 1 d . . . .
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H3B H 0.9158 0.5996 1.0222 0.057 Uiso 1 1 calc R U . . .
H3C H 0.9804 0.6817 1.0268 0.057 Uiso 1 1 calc R U . .
N4 N 0.88166(17) 0.77912(8) 0.72342(9) 0.0205(3) Uani 1 1 d . . . .
C5 C 0.9562(2) 0.82732(10) 0.70831(10) 0.0198(3) Uani 1 1 d . . . .
C6 C 1.0523(2) 0.88821(11) 0.68895(13) 0.0310(4) Uani 1 1 d . . . .
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C11 C 0.65561(17) 0.64947(8) 0.55068(9) 0.0118(3) Uani 1 1 d . . . .
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C12 C 0.51875(18) 0.64469(9) 0.50133(9) 0.0152(3) Uani 1 1 d . . . . H12 H 0.4330 0.6213 0.5197 0.018 Uiso 1 1 calc R U . . C13 C 0.5055(2) 0.67356(10) 0.42558(10) 0.0191(3) Uani 1 1 d . . . . H13 H 0.4117 0.6699 0.3927 0.023 Uiso 1 1 calc R U . . . C14 C 0.6305(2) 0.70770(10) 0.39871(10) 0.0196(3) Uani 1 1 d . . . . H14 H 0.6219 0.7275 0.3472 0.024 Uiso 1 1 calc R U . . . C15 C 0.76797(19) 0.71324(9) 0.44627(10) 0.0174(3) Uani 1 1 d . . . . H15 H 0.8529 0.7369 0.4274 0.021 Uiso 1 1 calc R U . . . C16 C 0.78122(18) 0.68385(8) 0.52197(9) 0.0134(3) Uani 1 1 d . . . . 017 0 0.91469(13) 0.68413(7) 0.57133(7) 0.0183(2) Uani 1 1 d . . . C18 C 1.03347(19) 0.73207(10) 0.55212(11) 0.0216(4) Uani 1 1 d . . . . H18A H 1.0759 0.7137 0.5054 0.032 Uiso 1 1 calc R U . . . H18B H 1.1144 0.7341 0.5962 0.032 Uiso 1 1 calc R U . . . H18C H 0.9916 0.7814 0.5416 0.032 Uiso 1 1 calc R U . . . C21 C 0.76123(16) 0.52412(8) 0.63995(9) 0.0119(3) Uani 1 1 d . . . . C22 C 0.80544(18) 0.50103(9) 0.56795(9) 0.0156(3) Uani 1 1 d . . . . H22 H 0.7827 0.5310 0.5228 0.019 Uiso 1 1 calc R U . . C23 C 0.8823(2) 0.43482(9) 0.56119(10) 0.0198(3) Uani 1 1 d . . . H23 H 0.9125 0.4201 0.5120 0.024 Uiso 1 1 calc R U . . . C24 C 0.9142(2) 0.39070(9) 0.62664(11) 0.0207(3) Uani 1 1 d . . . . H24 H 0.9664 0.3455 0.6222 0.025 Uiso 1 1 calc R U . . . C25 C 0.87059(18) 0.41182(9) 0.69892(10) 0.0171(3) Uani 1 1 d . . . . H25 H 0.8924 0.3811 0.7435 0.021 Uiso 1 1 calc R U . . . C26 C 0.79496(17) 0.47811(9) 0.70561(9) 0.0128(3) Uani 1 1 d . . . . 027 0 0.74721(14) 0.50218(7) 0.77499(7) 0.0181(2) Uani 1 1 d . . . . C28 C 0.8225(2) 0.47041(11) 0.84543(10) 0.0252(4) Uani 1 1 d . . . . H28A H 0.7997 0.4178 0.8465 0.038 Uiso 1 1 calc R U . . . H28B H 0.7862 0.4942 0.8912 0.038 Uiso 1 1 calc R U . . . H28C H 0.9332 0.4775 0.8468 0.038 Uiso 1 1 calc R U . . . C31 C 0.47532(17) 0.59075(9) 0.66420(9) 0.0121(3) Uani 1 1 d . . . . C32 C 0.41952(18) 0.52039(9) 0.64446(10) 0.0170(3) Uani 1 1 d . . . . H32 H 0.4848 0.4858 0.6235 0.020 Uiso 1 1 calc R U . . . C33 C 0.2708(2) 0.50010(10) 0.65484(11) 0.0242(4) Uani 1 1 d . . . . H33 H 0.2353 0.4521 0.6412 0.029 Uiso 1 1 calc R U . . C34 C 0.1748(2) 0.55006(11) 0.68512(12) 0.0277(4) Uani 1 1 d . . . . H34 H 0.0733 0.5363 0.6925 0.033 Uiso 1 1 calc R U . . . C35 C 0.22645(19) 0.62043(11) 0.70477(11) 0.0234(4) Uani 1 1 d . . . . H35 H 0.1598 0.6546 0.7254 0.028 Uiso 1 1 calc R U . . . C36 C 0.37560(17) 0.64127(9) 0.69436(9) 0.0148(3) Uani 1 1 d . . . . S1 S 0.43121(5) 0.73380(2) 0.71975(2) 0.01674(9) Uani 1 1 d . . . . O31 O 0.48470(16) 0.76530(7) 0.65014(7) 0.0250(3) Uani 1 1 d . . . . 032 0 0.29630(16) 0.76857(8) 0.74410(9) 0.0334(3) Uani 1 1 d . . . . O33 O 0.55389(14) 0.72726(7) 0.78518(7) 0.0210(3) Uani 1 1 d . . . C51 C 0.4826(4) 0.59093(14) 0.89333(15) 0.0495(6) Uani 1 1 d . . . . H51A H 0.5716 0.5985 0.9321 0.074 Uiso 1 1 calc R U . . . H51B H 0.4376 0.6385 0.8773 0.074 Uiso 1 1 calc R U . . . H51C H 0.5145 0.5657 0.8474 0.074 Uiso 1 1 calc R U . . . C52 C 0.3706(3) 0.54681(14) 0.92752(14) 0.0438(6) Uani 1 1 d . . . . N53 N 0.2851(3) 0.51145(17) 0.95512(17) 0.0721(8) Uani 1 1 d . . . .

loop

\_atom\_site\_aniso\_label \_atom\_site\_aniso\_U\_11 \_atom\_site\_aniso\_U\_22 \_atom\_site\_aniso\_U\_33 \_atom\_site\_aniso\_U\_23 \_atom\_site\_aniso\_U\_13 \_atom\_site\_aniso\_U\_12

Cul 0.01896(11) 0.01567(11) 0.01387(10) -0.00114(7) -0.00303(7) -0.00367(7)P1 0.00920(17) 0.00990(18) 0.00921(17) 0.00043(13) -0.00005(13) -0.00066(13)N1 0.0356(9) 0.0204(8) 0.0207(8) 0.0004(6) -0.0082(6) -0.0073(6) $C2 \ 0.0323(10) \ 0.0209(9) \ 0.0210(9) \ -0.0004(7) \ -0.0044(7) \ -0.0044(7)$ C3 0.0519(13) 0.0422(13) 0.0170(9) 0.0041(8) -0.0078(9) -0.0018(10) N4 0.0223(7) 0.0190(7) 0.0193(7) -0.0017(6) -0.0011(6) -0.0034(6)C5 0.0217(8) 0.0167(8) 0.0205(8) -0.0032(6) 0.0001(6) 0.0001(7) C6 0.0315(10) 0.0179(9) 0.0443(12) 0.0002(8) 0.0074(9) -0.0061(7) C11 0.0153(7) 0.0096(7) 0.0103(7) -0.0002(5) 0.0010(5) 0.0027(5) C12 0.0157(7) 0.0156(8) 0.0138(7) 0.0009(6) -0.0001(6) 0.0001(6) C13 0.0198(8) 0.0228(9) 0.0134(7) 0.0002(6) -0.0039(6) 0.0029(6) C14 0.0263(9) 0.0211(8) 0.0115(7) 0.0036(6) 0.0021(6) 0.0053(7) C15 0.0207(8) 0.0161(8) 0.0163(8) 0.0038(6) 0.0062(6) 0.0029(6) C16 0.0147(7) 0.0126(7) 0.0129(7) 0.0006(6) 0.0017(6) 0.0022(6) 017 0.0130(5) 0.0233(6) 0.0183(6) 0.0060(5) 0.0000(4) -0.0039(4) C18 0.0185(8) 0.0239(9) 0.0226(9) -0.0005(7) 0.0036(7) -0.0077(7) C21 0.0089(7) 0.0117(7) 0.0148(7) 0.0005(6) -0.0002(5) -0.0008(5) C22 0.0174(8) 0.0145(8) 0.0151(7) 0.0004(6) 0.0022(6) 0.0008(6) C23 0.0223(8) 0.0177(8) 0.0207(8) -0.0027(6) 0.0080(6) 0.0020(6) C24 0.0202(8) 0.0137(8) 0.0289(9) 0.0000(7) 0.0057(7) 0.0042(6) C25 0.0157(7) 0.0135(8) 0.0219(8) 0.0050(6) 0.0012(6) 0.0015(6) C26 0.0103(7) 0.0144(7) 0.0136(7) 0.0004(6) 0.0006(5) -0.0022(5)027 0.0245(6) 0.0189(6) 0.0112(5) 0.0032(4) 0.0031(4) 0.0038(5) C28 0.0359(10) 0.0237(9) 0.0147(8) 0.0054(7) -0.0028(7) 0.0006(8) C31 0.0109(7) 0.0142(7) 0.0109(7) 0.0019(5) -0.0005(5) -0.0012(5) C32 0.0156(8) 0.0152(8) 0.0195(8) 0.0007(6) -0.0022(6) -0.0023(6)C33 0.0177(8) 0.0222(9) 0.0310(10) 0.0031(7) -0.0046(7) -0.0091(7) C34 0.0117(8) 0.0344(11) 0.0370(11) 0.0065(8) 0.0023(7) -0.0078(7) C35 0.0145(8) 0.0292(10) 0.0271(9) 0.0038(7) 0.0054(7) 0.0024(7) C36 0.0130(7) 0.0165(8) 0.0150(7) 0.0027(6) 0.0017(6) 0.0003(6) S1 0.0187(2) 0.01416(19) 0.0183(2) -0.00118(15) 0.00623(15) 0.00314(14) 031 0.0372(7) 0.0174(6) 0.0214(6) 0.0037(5) 0.0082(5) 0.0000(5) 032 0.0266(7) 0.0297(8) 0.0460(9) -0.0100(6) 0.0139(6) 0.0095(6) 033 0.0261(6) 0.0190(6) 0.0179(6) -0.0038(5) 0.0023(5) -0.0017(5) C51 0.0783(19) 0.0353(13) 0.0386(13) 0.0073(10) 0.0236(12) 0.0010(12) C52 0.0631(16) 0.0377(13) 0.0334(12) 0.0047(10) 0.0188(11) 0.0119(11) N53 0.086(2) 0.0734(19) 0.0640(17) 0.0073(14) 0.0381(15) -0.0046(15) #\_\_\_\_\_\_ ---# # MOLECULAR GEOMETRY # # ----\_\_\_\_\_ ---# \_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 geom bond atom site label 2 geom bond distance geom bond site symmetry 2 \_geom\_bond\_publ\_flag Cul N1 1.9861(15) . ? Cul N4 1.9977(15) . ? Cul 033 2.2039(13) . ? Cul P1 2.2142(4) . ? P1 C11 1.8306(15) . ? P1 C21 1.8325(16) . ? P1 C31 1.8383(16) . ? N1 C2 1.137(2) . ? C2 C3 1.461(3) . ? C3 H3A 0.9800 . ? C3 H3B 0.9800 . ? C3 H3C 0.9800 . ? N4 C5 1.143(2) . ? C5 C6 1.455(3) . ? C6 H6A 0.9800 . ? C6 H6B 0.9800 . ? C6 H6C 0.9800 . ? C11 C12 1.396(2) . ? C11 C16 1.406(2) . ? C12 C13 1.394(2) . ? C12 H12 0.9500 . ? C13 C14 1.386(2) . ? C13 H13 0.9500 . ? C14 C15 1.386(2) . ? C14 H14 0.9500 . ? C15 C16 1.397(2) . ? C15 H15 0.9500 . ? C16 017 1.3700(19) . ? 017 C18 1.428(2) . ? C18 H18A 0.9800 . ? C18 H18B 0.9800 . ? C18 H18C 0.9800 . ? C21 C22 1.399(2) . ? C21 C26 1.409(2) . ? C22 C23 1.394(2) . ? C22 H22 0.9500 . ? C23 C24 1.384(3) . ? C23 H23 0.9500 . ? C24 C25 1.391(2) . ? C24 H24 0.9500 . ? C25 C26 1.390(2) . ? C25 H25 0.9500 . ? C26 O27 1.3761(19) . ? 027 C28 1.434(2) . ? C28 H28A 0.9800 . ? C28 H28B 0.9800 . ? C28 H28C 0.9800 . ? C31 C32 1.401(2) . ?

C31 C36 1.409(2) . ?

C32 C33 1.390(2) . ? C32 H32 0.9500 . ? C33 C34 1.381(3) . ? C33 H33 0.9500 . ? C34 C35 1.390(3) . ? C34 H34 0.9500 . ? C35 C36 1.397(2) . ? C35 H35 0.9500 . ? C36 S1 1.7962(17) . ? S1 032 1.4472(13) . ? S1 031 1.4487(13) . ? S1 033 1.4736(13) . ? C51 C52 1.445(4) . ? C51 H51A 0.9800 . ? C51 H51B 0.9800 . ? C51 H51C 0.9800 . ? C52 N53 1.133(4) . ? loop \_geom\_angle\_atom\_site label 1 \_geom\_angle\_atom\_site\_label\_2 \_geom\_angle\_atom\_site label 3 \_geom\_angle \_geom\_angle\_site\_symmetry 1 \_geom\_angle\_site\_symmetry\_3 geom angle publ flag N1 Cu1 N4 104.92(6) . . ? N1 Cu1 O33 95.45(6) . . ? N4 Cul 033 104.18(6) . . ? N1 Cu1 P1 126.90(5) . . ? N4 Cu1 P1 120.57(4) . . ? O33 Cu1 P1 98.26(3) . . ? C11 P1 C21 102.07(7) . . ? C11 P1 C31 101.99(7) . . ? C21 P1 C31 102.61(7) . . ? C11 P1 Cu1 118.38(5) . . ? C21 P1 Cu1 119.29(5) . . ? C31 P1 Cu1 110.10(5) . . ? C2 N1 Cu1 172.96(16) . . ? N1 C2 C3 179.7(3) . . ? C2 C3 H3A 109.5 . . ? C2 C3 H3B 109.5 . . ? H3A C3 H3B 109.5 . . ? C2 C3 H3C 109.5 . . ? H3A C3 H3C 109.5 . . ? H3B C3 H3C 109.5 . . ? C5 N4 Cu1 173.57(15) . . ? N4 C5 C6 179.5(2) . . ? C5 C6 H6A 109.5 . . ? С5 С6 Н6В 109.5 . . ? H6A C6 H6B 109.5 . . ? C5 C6 H6C 109.5 . . ? H6A C6 H6C 109.5 . . ? H6B C6 H6C 109.5 . . ? C12 C11 C16 118.33(14) . . ? C12 C11 P1 122.05(12) . . ? C16 C11 P1 119.61(11) . . ? C13 C12 C11 121.26(15) . . ?

C13 C12 H12 119.4 . . ? C11 C12 H12 119.4 . . ? C14 C13 C12 119.43(15) . . ? C14 C13 H13 120.3 . . ? C12 C13 H13 120.3 . . ? C13 C14 C15 120.68(15) . . ? C13 C14 H14 119.7 . . ? C15 C14 H14 119.7 . . ? C14 C15 C16 119.79(15) . . ? C14 C15 H15 120.1 . . ? C16 C15 H15 120.1 . . ? 017 C16 C15 123.41(14) . . ? 017 C16 C11 116.04(13) . . ? C15 C16 C11 120.51(15) . . ? C16 017 C18 117.35(13) . . ? 017 C18 H18A 109.5 . . ? 017 C18 H18B 109.5 . . ? H18A C18 H18B 109.5 . . ? 017 C18 H18C 109.5 . . ? H18A C18 H18C 109.5 . . ? H18B C18 H18C 109.5 . . ? C22 C21 C26 118.12(14) . . C22 C21 P1 121.56(12) . . ? C26 C21 P1 120.18(12) . . ? C23 C22 C21 121.20(15) . . ? C23 C22 H22 119.4 . . ? C21 C22 H22 119.4 . . ? C24 C23 C22 119.50(16) . . ? C24 C23 H23 120.2 . . ? C22 C23 H23 120.2 . . ? C23 C24 C25 120.68(15) . . ? C23 C24 H24 119.7 . . ? C25 C24 H24 119.7 . . ? C26 C25 C24 119.69(15) . . ? C26 C25 H25 120.2 . . ? C24 C25 H25 120.2 . . ? O27 C26 C25 122.88(14) . . ? 027 C26 C21 116.31(14) . . ? C25 C26 C21 120.81(14) . . ? C26 O27 C28 116.25(13) . . ? 027 C28 H28A 109.5 . . ? 027 C28 H28B 109.5 . . ? H28A C28 H28B 109.5 . . ? 027 C28 H28C 109.5 . . ? H28A C28 H28C 109.5 . . ? H28B C28 H28C 109.5 . . ? C32 C31 C36 118.09(14) . . ? C32 C31 P1 119.82(12) . . ? C36 C31 P1 122.09(12) . . ? C33 C32 C31 121.49(16) . . ? C33 C32 H32 119.3 . . ? СЗ1 СЗ2 НЗ2 119.3 . . ? C34 C33 C32 119.72(17) . . ? C34 C33 H33 120.1 . . ? СЗ2 СЗЗ НЗЗ 120.1 . . ? C33 C34 C35 120.16(16) . . ? C33 C34 H34 119.9 . . ? C35 C34 H34 119.9 . . ?

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C34 C35 H35 119.8 . . ?
C36 C35 H35 119.8 . . ?
C35 C36 C31 120.08(16) . . ?
C35 C36 S1 117.34(13) . . ?
C31 C36 S1 122.57(12) . . ?
O32 S1 O31 114.54(9) . . ?
O32 S1 O33 111.80(8) . . ?
O31 S1 O33 112.45(8) . .
                        ?
O32 S1 C36 105.71(8) . .
                        ?
O31 S1 C36 106.08(8) . .
                        ?
O33 S1 C36 105.41(7) . .
                        ?
S1 033 Cu1 112.77(7) . . ?
C52 C51 H51A 109.5 . . ?
C52 C51 H51B 109.5 . . ?
H51A C51 H51B 109.5 . . ?
C52 C51 H51C 109.5 . . ?
H51A C51 H51C 109.5 . . ?
H51B C51 H51C 109.5 . . ?
N53 C52 C51 178.6(3) . . ?
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geom torsion atom site label 2
_geom_torsion_atom_site_label_3
geom torsion atom site label 4
geom torsion
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geom torsion site symmetry 2
_geom_torsion_site_symmetry 3
_geom_torsion_site symmetry 4
geom torsion publ flag
C21 P1 C11 C12 97.74(14) . . . ?
C31 P1 C11 C12 -8.14(15) . . . ?
Cul P1 C11 C12 -129.08(12) . . .
C21 P1 C11 C16 -83.59(13) . . . ?
C31 P1 C11 C16 170.53(12) . . . ?
Cul P1 C11 C16 49.59(14) . . . ?
C16 C11 C12 C13 -0.4(2) . . . ?
P1 C11 C12 C13 178.24(13) . . . ?
C11 C12 C13 C14 0.0(3) . . . ?
C12 C13 C14 C15 0.1(3) . . . ?
C13 C14 C15 C16 0.3(3) . . . ?
C14 C15 C16 O17 177.01(15) . . . ?
C14 C15 C16 C11 -0.8(2) . . . ?
C12 C11 C16 O17 -177.11(14) . . . ?
P1 C11 C16 O17 4.17(19) . . . ?
C12 C11 C16 C15 0.9(2) . . . ?
P1 C11 C16 C15 -177.86(12) . . .
C15 C16 O17 C18 15.9(2) . . . ?
C11 C16 O17 C18 -166.25(14) . . . ?
C11 P1 C21 C22 4.46(14) . . . ?
C31 P1 C21 C22 109.86(13) . . . ?
Cul P1 C21 C22 -128.18(12) . . . ?
C11 P1 C21 C26 -179.93(12) . . . ?
C31 P1 C21 C26 -74.53(13) . . . ?
Cu1 P1 C21 C26 47.43(14) . . . ?
C26 C21 C22 C23 -0.7(2) . . . ?
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P1 C21 C22 C23 174.98(13) . . . ?
C21 C22 C23 C24 0.6(3) . . . ?
C22 C23 C24 C25 -0.1(3) . . . ?
C23 C24 C25 C26 -0.4(3) . . . ?
C24 C25 C26 O27 179.37(15) . . . ?
C24 C25 C26 C21 0.3(2) . . . ?
C22 C21 C26 O27 -178.90(13) . . . ?
P1 C21 C26 O27 5.34(19) . . . ?
C22 C21 C26 C25 0.3(2) . . . ?
P1 C21 C26 C25 -175.51(12) . . . ?
C25 C26 O27 C28 21.1(2) . . . ?
C21 C26 O27 C28 -159.75(14) . . . ?
C11 P1 C31 C32 89.81(13) . . . ?
C21 P1 C31 C32 -15.65(14) . . . ?
Cul P1 C31 C32 -143.66(11) . . . ?
C11 P1 C31 C36 -90.82(13) . . . ?
C21 P1 C31 C36 163.72(13) . . . ?
Cu1 P1 C31 C36 35.71(14) . . . ?
C36 C31 C32 C33 -0.7(2) . . . ?
P1 C31 C32 C33 178.72(13) . . . ?
C31 C32 C33 C34 0.1(3) . . . ?
C32 C33 C34 C35 0.3(3) . . . ?
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C34 C35 C36 C31 -0.4(3) . . . ?
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C32 C31 C36 S1 -178.48(12) . . . .
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C31 C36 S1 O32 177.01(13) . . . ?
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C31 C36 S1 O31 55.00(15) . . . ?
C35 C36 S1 O33 116.26(14) . . . ?
C31 C36 S1 O33 -64.45(15) . . . ?
O32 S1 O33 Cu1 -172.68(8) . . . ?
O31 S1 O33 Cu1 -42.20(9) . . . ?
C36 S1 O33 Cu1 72.94(8) . . . ?
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