

data\_paratimroseite

\_audit\_creation\_method SHELXL-97

\_chemical\_name\_systematic

;

?

;

\_chemical\_name\_common ?

\_chemical\_melting\_point ?

\_chemical\_formula\_moiety ?

\_chemical\_formula\_sum

'H2 Cu2 O7 Pb Te'

\_chemical\_formula\_weight 575.89

loop\_

\_atom\_type\_symbol

\_atom\_type\_description

\_atom\_type\_scatter\_dispersion\_real

\_atom\_type\_scatter\_dispersion\_imag

\_atom\_type\_scatter\_source

'Pb' 'Pb' -3.3944 10.1111

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Te' 'Te' -0.5308 1.6751

'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'

'O' 'O' 0.0106 0.0060

'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'

\_symmetry\_cell\_setting ?

\_symmetry\_space\_group\_name\_H-M ?

loop\_

\_symmetry\_equiv\_pos\_as\_xyz

'x, y, z'

'x+1/2, -y+1/2, -z'

'-x, y+1/2, -z+1/2'

'-x+1/2, -y, z+1/2'

\_cell\_length\_a 5.1943(4)

\_cell\_length\_b 9.6198(10)

\_cell\_length\_c 11.6745(11)

\_cell\_angle\_alpha 90.00

\_cell\_angle\_beta 90.00

\_cell\_angle\_gamma 90.00

\_cell\_volume 583.35(9)

\_cell\_formula\_units\_Z 4

\_cell\_measurement\_temperature 293(2)

\_cell\_measurement\_reflns\_used ?

\_cell\_measurement\_theta\_min ?

```

_cell_measurement_theta_max      ?

_exptl_crystal_description      ?
_exptl_crystal_colour           ?
_exptl_crystal_size_max         0.05
_exptl_crystal_size_mid         0.03
_exptl_crystal_size_min         0.01
_exptl_crystal_density_meas     ?
_exptl_crystal_density_diffn    6.557
_exptl_crystal_density_method   'not measured'
_exptl_crystal_F_000            1000
_exptl_absorpt_coefficient_mu    40.901
_exptl_absorpt_correction_type  ?
_exptl_absorpt_correction_T_min 0.2605
_exptl_absorpt_correction_T_max 0.7914
_exptl_absorpt_process_details  ?

_exptl_special_details
;
?
;

_diffrn_ambient_temperature      293(2)
_diffrn_radiation_wavelength     0.71075
_diffrn_radiation_type           MoK\alpha
_diffrn_radiation_source         'fine-focus sealed tube'
_diffrn_radiation_monochromator  graphite
_diffrn_measurement_device_type  ?
_diffrn_measurement_method       ?
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number         ?
_diffrn_standards_interval_count ?
_diffrn_standards_interval_time  ?
_diffrn_standards_decay_%        ?
_diffrn_reflns_number            4431
_diffrn_reflns_av_R_equivalents  0.1114
_diffrn_reflns_av_sigmaI/netI    0.0884
_diffrn_reflns_limit_h_min       -5
_diffrn_reflns_limit_h_max       6
_diffrn_reflns_limit_k_min       -11
_diffrn_reflns_limit_k_max       11
_diffrn_reflns_limit_l_min       -13
_diffrn_reflns_limit_l_max       13
_diffrn_reflns_theta_min         3.49
_diffrn_reflns_theta_max         24.70
_reflns_number_total             984
_reflns_number_gt                842
_reflns_threshold_expression      >2sigma(I)

_computing_data_collection       ?
_computing_cell_refinement       ?
_computing_data_reduction        ?
_computing_structure_solution    'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'

```

\_computing\_molecular\_graphics ?  
\_computing\_publication\_material ?

\_refine\_special\_details

;

Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and goodness of fit S are based on  $F^2$ , conventional R-factors R are based on F, with F set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

;

\_refine\_ls\_structure\_factor\_coef Fsqd  
\_refine\_ls\_matrix\_type full  
\_refine\_ls\_weighting\_scheme calc  
\_refine\_ls\_weighting\_details  
'calc w=1/[\s^2^(Fo^2^)+(0.0000P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'  
\_atom\_sites\_solution\_primary direct  
\_atom\_sites\_solution\_secondary difmap  
\_atom\_sites\_solution\_hydrogens geom  
\_refine\_ls\_hydrogen\_treatment mixed  
\_refine\_ls\_extinction\_method none  
\_refine\_ls\_extinction\_coef ?  
\_refine\_ls\_abs\_structure\_details  
'Flack H D (1983), Acta Cryst. A39, 876-881'  
\_refine\_ls\_abs\_structure\_Flack 0.018(16)  
\_refine\_ls\_number\_reflns 984  
\_refine\_ls\_number\_parameters 91  
\_refine\_ls\_number\_restraints 0  
\_refine\_ls\_R\_factor\_all 0.0500  
\_refine\_ls\_R\_factor\_gt 0.0388  
\_refine\_ls\_wR\_factor\_ref 0.0783  
\_refine\_ls\_wR\_factor\_gt 0.0731  
\_refine\_ls\_goodness\_of\_fit\_ref 0.974  
\_refine\_ls\_restrained\_S\_all 0.974  
\_refine\_ls\_shift/su\_max 0.002  
\_refine\_ls\_shift/su\_mean 0.000

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\_symmetry\_multiplicity  
\_atom\_site\_calc\_flag  
\_atom\_site\_refinement\_flags  
\_atom\_site\_disorder\_assembly  
\_atom\_site\_disorder\_group

Pb Pb 0.48658(16) 0.37646(9) 0.71849(6) 0.0199(2) Uani 1 1 d . . .  
 Te Te 0.8986(2) 0.49499(15) 0.49034(11) 0.0124(3) Uani 1 1 d . . .  
 Cu1 Cu 0.3802(4) 0.6442(3) 0.5457(2) 0.0148(6) Uani 1 1 d . . .  
 Cu2 Cu 0.4205(4) 0.3513(3) 0.4222(2) 0.0145(6) Uani 1 1 d . . .  
 O1 O 0.608(3) 0.5291(15) 0.3914(11) 0.016(3) Uani 1 1 d . . .  
 O2 O 0.195(3) 0.4730(15) 0.5870(11) 0.012(3) Uiso 1 1 d . . .  
 O3 O 0.544(3) 0.8222(14) 0.5322(11) 0.023(4) Uiso 1 1 d . . .  
 O4 O 0.741(3) 0.3179(14) 0.5188(12) 0.022(4) Uani 1 1 d . . .  
 O5 O 0.415(3) 0.5715(15) 0.8624(11) 0.017(4) Uani 1 1 d . . .  
 O6 O 0.696(3) 0.5660(16) 0.6193(11) 0.019(4) Uani 1 1 d . . .  
 OW O 0.473(3) 0.7477(14) 0.2604(10) 0.024(4) 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  
 Pb 0.0182(4) 0.0224(5) 0.0192(4) 0.0041(4) 0.0004(4) 0.0012(5)  
 Te 0.0100(6) 0.0117(7) 0.0155(7) -0.0003(6) -0.0003(5) 0.0000(6)  
 Cu1 0.0090(12) 0.0157(15) 0.0196(14) 0.0012(11) -0.0011(9) 0.0007(12)  
 Cu2 0.0090(13) 0.0159(15) 0.0184(14) 0.0005(11) -0.0015(10) -0.0012(11)  
 O1 0.018(8) 0.015(8) 0.016(8) 0.002(6) -0.012(6) -0.007(7)  
 O4 0.018(8) 0.007(8) 0.041(10) 0.005(7) 0.003(7) -0.010(6)  
 O5 0.007(8) 0.032(10) 0.012(8) -0.003(6) 0.000(5) 0.000(7)  
 O6 0.018(8) 0.028(10) 0.011(8) -0.002(6) 0.010(6) 0.001(7)  
 OW 0.043(10) 0.008(8) 0.020(8) -0.005(6) 0.008(7) -0.003(8)

\_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  
 Pb O2 2.348(13) . ?  
 Pb O6 2.419(14) . ?  
 Pb O5 2.546(13) . ?  
 Pb OW 2.714(17) 4\_565 ?  
 Pb O4 2.737(15) . ?  
 Pb O3 2.962(13) 3\_646 ?  
 Pb O1 3.055(15) 4\_665 ?  
 Pb OW 3.090(17) 4\_665 ?

Pb O5 3.124(14) 3\_646 ?  
 Pb Cu1 3.318(3) . ?  
 Pb Te 3.4579(15) 4\_665 ?  
 Pb Cu2 3.484(3) . ?  
 Pb Cu2 3.547(2) 2\_556 ?  
 Pb O4 3.578(15) 2\_456 ?  
 Pb Te 3.6022(15) . ?  
 Pb Cu1 3.613(3) 3\_646 ?  
 Pb O6 3.662(15) 3\_646 ?  
 Pb O1 3.799(13) 4\_565 ?  
 Pb Cu2 4.018(2) 2\_456 ?  
 Pb O2 4.093(13) 1\_655 ?  
 Te O5 1.892(13) 4\_664 ?  
 Te O2 1.920(13) 1\_655 ?  
 Te O4 1.920(13) . ?  
 Te O3 1.932(14) 2\_566 ?  
 Te O1 1.929(13) . ?  
 Te O6 1.959(13) . ?  
 Te Cu2 2.952(3) . ?  
 Te Cu1 2.955(3) 1\_655 ?  
 Te Cu1 3.119(3) . ?  
 Te Cu2 3.145(3) 1\_655 ?  
 Te Pb 3.4580(15) 4\_664 ?  
 Te Cu2 3.486(3) 2\_556 ?  
 Cu1 O3 1.919(14) . ?  
 Cu1 O2 1.967(14) . ?  
 Cu1 O3 1.995(14) 2\_466 ?  
 Cu1 O6 2.000(15) . ?  
 Cu1 O1 2.423(15) . ?  
 Cu1 Te 2.955(3) 1\_455 ?  
 Cu2 O4 1.999(14) 2\_456 ?  
 Cu2 O1 2.001(15) . ?  
 Cu2 O5 2.018(13) 4\_564 ?  
 Cu2 O4 2.034(14) . ?  
 Cu2 OW 2.418(13) 3\_645 ?  
 Cu2 O2 2.539(13) . ?  
 O1 OW 2.693(19) . ?  
 O1 Pb 3.055(14) 4\_664 ?  
 O1 Cu1 3.524(14) 2\_566 ?  
 O1 Pb 3.799(13) 4\_564 ?  
 O2 Te 1.920(13) 1\_455 ?  
 O2 Cu2 3.432(14) 2\_456 ?  
 O2 Pb 4.093(13) 1\_455 ?  
 O3 Te 1.932(14) 2\_466 ?  
 O3 Cu1 1.995(14) 2\_566 ?  
 O3 Pb 2.962(13) 3\_656 ?  
 O3 Cu1 3.580(13) 2\_466 ?  
 O3 Cu2 3.738(14) 2\_566 ?  
 O4 Cu2 1.999(14) 2\_556 ?  
 O4 Pb 3.578(15) 2\_556 ?  
 O4 Cu2 3.721(13) 1\_655 ?  
 O5 Te 1.892(13) 4\_665 ?  
 O5 Cu2 2.018(13) 4\_565 ?  
 O5 Pb 3.124(14) 3\_656 ?

O5 Cu1 3.351(14) 4\_565 ?  
O5 Cu2 3.600(14) 4\_665 ?  
O5 Cu2 3.781(14) 3\_656 ?  
O6 Cu1 3.520(14) 2\_566 ?  
O6 Pb 3.662(14) 3\_656 ?  
O6 Cu1 3.731(14) 1\_655 ?  
O6 Cu2 4.136(14) 4\_665 ?  
O6 OW 4.685(19) . ?  
OW Cu2 2.418(13) 3\_655 ?  
OW Pb 2.714(17) 4\_564 ?  
OW Pb 3.090(17) 4\_664 ?  
OW Cu1 3.268(16) 2\_566 ?  
OW Cu1 3.960(15) 2\_466 ?

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  
O2 Pb O6 71.3(5) . . ?  
O2 Pb O5 92.6(5) . . ?  
O6 Pb O5 80.0(5) . . ?  
O2 Pb OW 74.0(4) . 4\_565 ?  
O6 Pb OW 144.5(5) . 4\_565 ?  
O5 Pb OW 94.4(4) . 4\_565 ?  
O2 Pb O4 80.5(4) . . ?  
O6 Pb O4 62.0(4) . . ?  
O5 Pb O4 141.7(4) . . ?  
OW Pb O4 119.1(4) 4\_565 . ?  
O2 Pb O3 132.6(4) . 3\_646 ?  
O6 Pb O3 128.9(4) . 3\_646 ?  
O5 Pb O3 58.2(4) . 3\_646 ?  
OW Pb O3 72.4(4) 4\_565 3\_646 ?  
O4 Pb O3 145.8(4) . 3\_646 ?  
O2 Pb O1 139.4(4) . 4\_665 ?  
O6 Pb O1 77.4(4) . 4\_665 ?  
O5 Pb O1 56.3(4) . 4\_665 ?  
OW Pb O1 128.2(4) 4\_565 4\_665 ?  
O4 Pb O1 107.0(4) . 4\_665 ?  
O3 Pb O1 55.9(3) 3\_646 4\_665 ?  
O2 Pb OW 147.4(4) . 4\_665 ?  
O6 Pb OW 87.6(5) . 4\_665 ?  
O5 Pb OW 108.3(4) . 4\_665 ?  
OW Pb OW 126.9(5) 4\_565 4\_665 ?  
O4 Pb OW 67.5(4) . 4\_665 ?  
O3 Pb OW 79.9(4) 3\_646 4\_665 ?  
O1 Pb OW 52.0(4) 4\_665 4\_665 ?  
O2 Pb O5 106.2(4) . 3\_646 ?  
O6 Pb O5 119.3(4) . 3\_646 ?  
O5 Pb O5 156.3(3) . 3\_646 ?  
OW Pb O5 77.6(4) 4\_565 3\_646 ?

O4 Pb O5 58.0(4) . 3\_646 ?  
 O3 Pb O5 98.1(4) 3\_646 3\_646 ?  
 O1 Pb O5 111.5(4) 4\_665 3\_646 ?  
 OW Pb O5 62.4(4) 4\_665 3\_646 ?  
 O2 Pb Cu1 35.7(3) . . ?  
 O6 Pb Cu1 36.8(4) . . ?  
 O5 Pb Cu1 78.8(3) . . ?  
 OW Pb Cu1 107.8(3) 4\_565 . ?  
 O4 Pb Cu1 73.9(3) . . ?  
 O3 Pb Cu1 136.5(3) 3\_646 . ?  
 O1 Pb Cu1 106.6(3) 4\_665 . ?  
 OW Pb Cu1 123.2(3) 4\_665 . ?  
 O5 Pb Cu1 124.9(2) 3\_646 . ?  
 O2 Pb Te 124.7(3) . 4\_665 ?  
 O6 Pb Te 95.3(3) . 4\_665 ?  
 O5 Pb Te 32.4(3) . 4\_665 ?  
 OW Pb Te 98.2(3) 4\_565 4\_665 ?  
 O4 Pb Te 140.6(3) . 4\_665 ?  
 O3 Pb Te 33.9(3) 3\_646 4\_665 ?  
 O1 Pb Te 33.7(2) 4\_665 4\_665 ?  
 OW Pb Te 80.6(2) 4\_665 4\_665 ?  
 O5 Pb Te 125.8(2) 3\_646 4\_665 ?  
 Cu1 Pb Te 108.02(5) . 4\_665 ?  
 O2 Pb Cu2 46.8(3) . . ?  
 O6 Pb Cu2 67.8(3) . . ?  
 O5 Pb Cu2 133.8(3) . . ?  
 OW Pb Cu2 93.5(3) 4\_565 . ?  
 O4 Pb Cu2 35.7(3) . . ?  
 O3 Pb Cu2 163.4(3) 3\_646 . ?  
 O1 Pb Cu2 138.1(2) 4\_665 . ?  
 OW Pb Cu2 102.7(2) 4\_665 . ?  
 O5 Pb Cu2 69.6(2) 3\_646 . ?  
 Cu1 Pb Cu2 55.52(6) . . ?  
 Te Pb Cu2 162.36(6) 4\_665 . ?  
 O2 Pb Cu2 110.6(3) . 2\_556 ?  
 O6 Pb Cu2 87.6(3) . 2\_556 ?  
 O5 Pb Cu2 148.6(3) . 2\_556 ?  
 OW Pb Cu2 111.8(3) 4\_565 2\_556 ?  
 O4 Pb Cu2 34.1(3) . 2\_556 ?  
 O3 Pb Cu2 112.4(3) 3\_646 2\_556 ?  
 O1 Pb Cu2 93.0(3) 4\_665 2\_556 ?  
 OW Pb Cu2 42.0(2) 4\_665 2\_556 ?  
 O5 Pb Cu2 34.5(2) 3\_646 2\_556 ?  
 Cu1 Pb Cu2 107.67(6) . 2\_556 ?  
 Te Pb Cu2 122.45(5) 4\_665 2\_556 ?  
 Cu2 Pb Cu2 63.88(5) . 2\_556 ?  
 O2 Pb O4 58.0(4) . 2\_456 ?  
 O6 Pb O4 100.6(4) . 2\_456 ?  
 O5 Pb O4 147.5(4) . 2\_456 ?  
 OW Pb O4 66.1(4) 4\_565 2\_456 ?  
 O4 Pb O4 53.50(18) . 2\_456 ?  
 O3 Pb O4 130.5(4) 3\_646 2\_456 ?  
 O1 Pb O4 155.9(3) 4\_665 2\_456 ?  
 OW Pb O4 104.2(3) 4\_665 2\_456 ?

O5 Pb O4 48.2(3) 3\_646 2\_456 ?  
 Cu1 Pb O4 82.8(2) . 2\_456 ?  
 Te Pb O4 163.5(2) 4\_665 2\_456 ?  
 Cu2 Pb O4 32.9(2) . 2\_456 ?  
 Cu2 Pb O4 63.0(2) 2\_556 2\_456 ?  
 O2 Pb Te 77.0(3) . . ?  
 O6 Pb Te 30.7(3) . . ?  
 O5 Pb Te 110.0(3) . . ?  
 OW Pb Te 142.7(3) 4\_565 . ?  
 O4 Pb Te 31.7(3) . . ?  
 O3 Pb Te 144.5(3) 3\_646 . ?  
 O1 Pb Te 89.1(2) 4\_665 . ?  
 OW Pb Te 72.5(3) 4\_665 . ?  
 O5 Pb Te 88.6(2) 3\_646 . ?  
 Cu1 Pb Te 53.39(5) . . ?  
 Te Pb Te 117.58(2) 4\_665 . ?  
 Cu2 Pb Te 49.20(4) . . ?  
 Cu2 Pb Te 58.36(5) 2\_556 . ?  
 O4 Pb Te 78.8(2) 2\_456 . ?  
 O2 Pb Cu1 150.0(3) . 3\_646 ?  
 O6 Pb Cu1 138.1(3) . 3\_646 ?  
 O5 Pb Cu1 88.9(3) . 3\_646 ?  
 OW Pb Cu1 76.0(3) 4\_565 3\_646 ?  
 O4 Pb Cu1 115.4(3) . 3\_646 ?  
 O3 Pb Cu1 32.0(3) 3\_646 3\_646 ?  
 O1 Pb Cu1 63.2(3) 4\_665 3\_646 ?  
 OW Pb Cu1 57.7(3) 4\_665 3\_646 ?  
 O5 Pb Cu1 67.6(2) 3\_646 3\_646 ?  
 Cu1 Pb Cu1 167.26(7) . 3\_646 ?  
 Te Pb Cu1 59.25(5) 4\_665 3\_646 ?  
 Cu2 Pb Cu1 137.09(7) . 3\_646 ?  
 Cu2 Pb Cu1 81.33(6) 2\_556 3\_646 ?  
 O4 Pb Cu1 109.6(2) 2\_456 3\_646 ?  
 Te Pb Cu1 130.20(5) . 3\_646 ?  
 O2 Pb O6 119.5(4) . 3\_646 ?  
 O6 Pb O6 168.3(2) . 3\_646 ?  
 O5 Pb O6 102.8(4) . 3\_646 ?  
 OW Pb O6 47.1(4) 4\_565 3\_646 ?  
 O4 Pb O6 113.4(4) . 3\_646 ?  
 O3 Pb O6 48.2(3) 3\_646 3\_646 ?  
 O1 Pb O6 94.6(3) 4\_665 3\_646 ?  
 OW Pb O6 80.7(4) 4\_665 3\_646 ?  
 O5 Pb O6 55.5(3) 3\_646 3\_646 ?  
 Cu1 Pb O6 154.7(2) . 3\_646 ?  
 Te Pb O6 82.0(2) 4\_665 3\_646 ?  
 Cu2 Pb O6 115.5(2) . 3\_646 ?  
 Cu2 Pb O6 84.3(2) 2\_556 3\_646 ?  
 O4 Pb O6 83.2(3) 2\_456 3\_646 ?  
 Te Pb O6 142.6(2) . 3\_646 ?  
 Cu1 Pb O6 31.9(2) 3\_646 3\_646 ?  
 O2 Pb O1 74.2(4) . 4\_565 ?  
 O6 Pb O1 116.1(4) . 4\_565 ?  
 O5 Pb O1 49.8(4) . 4\_565 ?  
 OW Pb O1 45.1(4) 4\_565 4\_565 ?

O4 Pb O1 153.3(4) . 4\_565 ?  
 O3 Pb O1 58.4(3) 3\_646 4\_565 ?  
 O1 Pb O1 97.9(3) 4\_665 4\_565 ?  
 OW Pb O1 138.3(3) 4\_665 4\_565 ?  
 O5 Pb O1 121.2(3) 3\_646 4\_565 ?  
 Cu1 Pb O1 90.1(2) . 4\_565 ?  
 Te Pb O1 64.3(2) 4\_665 4\_565 ?  
 Cu2 Pb O1 117.6(2) . 4\_565 ?  
 Cu2 Pb O1 155.5(2) 2\_556 4\_565 ?  
 O4 Pb O1 104.2(3) 2\_456 4\_565 ?  
 Te Pb O1 143.1(2) . 4\_565 ?  
 Cu1 Pb O1 84.2(2) 3\_646 4\_565 ?  
 O6 Pb O1 73.1(3) 3\_646 4\_565 ?  
 O2 Pb Cu2 58.4(3) . 2\_456 ?  
 O6 Pb Cu2 123.0(3) . 2\_456 ?  
 O5 Pb Cu2 124.4(3) . 2\_456 ?  
 OW Pb Cu2 35.9(3) 4\_565 2\_456 ?  
 O4 Pb Cu2 83.8(3) . 2\_456 ?  
 O3 Pb Cu2 105.5(3) 3\_646 2\_456 ?  
 O1 Pb Cu2 159.5(3) 4\_665 2\_456 ?  
 OW Pb Cu2 121.3(3) 4\_665 2\_456 ?  
 O5 Pb Cu2 59.0(3) 3\_646 2\_456 ?  
 Cu1 Pb Cu2 93.02(6) . 2\_456 ?  
 Te Pb Cu2 134.14(5) 4\_665 2\_456 ?  
 Cu2 Pb Cu2 58.94(5) . 2\_456 ?  
 Cu2 Pb Cu2 86.49(6) 2\_556 2\_456 ?  
 O4 Pb Cu2 30.4(2) 2\_456 2\_456 ?  
 Te Pb Cu2 107.76(4) . 2\_456 ?  
 Cu1 Pb Cu2 96.58(5) 3\_646 2\_456 ?  
 O6 Pb Cu2 65.0(2) 3\_646 2\_456 ?  
 O1 Pb Cu2 75.7(2) 4\_565 2\_456 ?  
 O2 Pb O2 104.2(4) . 1\_655 ?  
 O6 Pb O2 40.9(4) . 1\_655 ?  
 O5 Pb O2 102.2(4) . 1\_655 ?  
 OW Pb O2 163.4(4) 4\_565 1\_655 ?  
 O4 Pb O2 45.1(3) . 1\_655 ?  
 O3 Pb O2 117.2(3) 3\_646 1\_655 ?  
 O1 Pb O2 63.9(3) 4\_665 1\_655 ?  
 OW Pb O2 48.0(3) 4\_665 1\_655 ?  
 O5 Pb O2 87.3(3) 3\_646 1\_655 ?  
 Cu1 Pb O2 75.25(19) . 1\_655 ?  
 Te Pb O2 96.20(19) 4\_665 1\_655 ?  
 Cu2 Pb O2 74.47(18) . 1\_655 ?  
 Cu2 Pb O2 52.8(2) 2\_556 1\_655 ?  
 O4 Pb O2 98.6(3) 2\_456 1\_655 ?  
 Te Pb O2 27.97(18) . 1\_655 ?  
 Cu1 Pb O2 104.72(19) 3\_646 1\_655 ?  
 O6 Pb O2 127.8(3) 3\_646 1\_655 ?  
 O1 Pb O2 151.1(3) 4\_565 1\_655 ?  
 Cu2 Pb O2 128.92(19) 2\_456 1\_655 ?  
 O5 Te O2 90.9(6) 4\_664 1\_655 ?  
 O5 Te O4 93.2(6) 4\_664 . ?  
 O2 Te O4 98.3(6) 1\_655 . ?  
 O5 Te O3 90.0(6) 4\_664 2\_566 ?

O2 Te O3 82.4(6) 1\_655 2\_566 ?  
 O4 Te O3 176.7(6) . 2\_566 ?  
 O5 Te O1 89.2(6) 4\_664 . ?  
 O2 Te O1 176.4(6) 1\_655 . ?  
 O4 Te O1 85.4(6) . . ?  
 O3 Te O1 94.0(6) 2\_566 . ?  
 O5 Te O6 178.1(6) 4\_664 . ?  
 O2 Te O6 90.9(6) 1\_655 . ?  
 O4 Te O6 87.0(6) . . ?  
 O3 Te O6 89.8(6) 2\_566 . ?  
 O1 Te O6 88.9(6) . . ?  
 O5 Te Cu2 93.4(4) 4\_664 . ?  
 O2 Te Cu2 141.4(4) 1\_655 . ?  
 O4 Te Cu2 43.2(4) . . ?  
 O3 Te Cu2 135.9(4) 2\_566 . ?  
 O1 Te Cu2 42.2(4) . . ?  
 O6 Te Cu2 85.4(4) . . ?  
 O5 Te Cu1 84.4(4) 4\_664 1\_655 ?  
 O2 Te Cu1 41.1(4) 1\_655 1\_655 ?  
 O4 Te Cu1 139.0(4) . 1\_655 ?  
 O3 Te Cu1 42.0(4) 2\_566 1\_655 ?  
 O1 Te Cu1 135.3(4) . 1\_655 ?  
 O6 Te Cu1 96.7(4) . 1\_655 ?  
 Cu2 Te Cu1 176.92(9) . 1\_655 ?  
 O5 Te Cu1 139.6(4) 4\_664 . ?  
 O2 Te Cu1 128.4(4) 1\_655 . ?  
 O4 Te Cu1 90.2(4) . . ?  
 O3 Te Cu1 86.9(4) 2\_566 . ?  
 O1 Te Cu1 51.0(4) . . ?  
 O6 Te Cu1 38.5(4) . . ?  
 Cu2 Te Cu1 62.92(7) . . ?  
 Cu1 Te Cu1 117.52(10) 1\_655 . ?  
 O5 Te Cu2 37.8(4) 4\_664 1\_655 ?  
 O2 Te Cu2 53.8(4) 1\_655 1\_655 ?  
 O4 Te Cu2 91.3(4) . 1\_655 ?  
 O3 Te Cu2 91.7(4) 2\_566 1\_655 ?  
 O1 Te Cu2 126.7(4) . 1\_655 ?  
 O6 Te Cu2 144.1(4) . 1\_655 ?  
 Cu2 Te Cu2 116.82(10) . 1\_655 ?  
 Cu1 Te Cu2 62.56(7) 1\_655 1\_655 ?  
 Cu1 Te Cu2 177.13(8) . 1\_655 ?  
 O5 Te Pb 46.2(4) 4\_664 4\_664 ?  
 O2 Te Pb 116.2(4) 1\_655 4\_664 ?  
 O4 Te Pb 123.3(4) . 4\_664 ?  
 O3 Te Pb 58.8(4) 2\_566 4\_664 ?  
 O1 Te Pb 61.6(4) . 4\_664 ?  
 O6 Te Pb 132.3(4) . 4\_664 ?  
 Cu2 Te Pb 93.75(6) . 4\_664 ?  
 Cu1 Te Pb 83.17(6) 1\_655 4\_664 ?  
 Cu1 Te Pb 100.04(6) . 4\_664 ?  
 Cu2 Te Pb 77.09(5) 1\_655 4\_664 ?  
 O5 Te Cu2 83.8(4) 4\_664 2\_556 ?  
 O2 Te Cu2 72.3(4) 1\_655 2\_556 ?  
 O4 Te Cu2 27.8(4) . 2\_556 ?

O3 Te Cu2 153.8(4) 2\_566 2\_556 ?  
 O1 Te Cu2 111.3(4) . 2\_556 ?  
 O6 Te Cu2 97.2(4) . 2\_556 ?  
 Cu2 Te Cu2 70.04(6) . 2\_556 ?  
 Cu1 Te Cu2 111.87(8) 1\_655 2\_556 ?  
 Cu1 Te Cu2 114.02(7) . 2\_556 ?  
 Cu2 Te Cu2 68.03(6) 1\_655 2\_556 ?  
 Pb Te Cu2 127.22(6) 4\_664 2\_556 ?  
 O3 Cu1 O2 169.7(6) . . ?  
 O3 Cu1 O3 101.9(4) . 2\_466 ?  
 O2 Cu1 O3 79.6(6) . 2\_466 ?  
 O3 Cu1 O6 90.4(6) . . ?  
 O2 Cu1 O6 89.0(6) . . ?  
 O3 Cu1 O6 167.2(6) 2\_466 . ?  
 O3 Cu1 O1 97.5(5) . . ?  
 O2 Cu1 O1 92.2(5) . . ?  
 O3 Cu1 O1 99.4(5) 2\_466 . ?  
 O6 Cu1 O1 75.3(5) . . ?  
 O3 Cu1 Te 142.2(4) . 1\_455 ?  
 O2 Cu1 Te 39.9(4) . 1\_455 ?  
 O3 Cu1 Te 40.4(4) 2\_466 1\_455 ?  
 O6 Cu1 Te 127.3(4) . 1\_455 ?  
 O1 Cu1 Te 91.7(3) . 1\_455 ?  
 O4 Cu2 O1 170.2(6) 2\_456 . ?  
 O4 Cu2 O5 90.9(6) 2\_456 4\_564 ?  
 O1 Cu2 O5 92.5(6) . 4\_564 ?  
 O4 Cu2 O4 93.6(3) 2\_456 . ?  
 O1 Cu2 O4 80.6(5) . . ?  
 O5 Cu2 O4 162.8(6) 4\_564 . ?  
 O4 Cu2 OW 94.3(5) 2\_456 3\_645 ?  
 O1 Cu2 OW 94.7(5) . 3\_645 ?  
 O5 Cu2 OW 92.5(6) 4\_564 3\_645 ?  
 O4 Cu2 OW 103.7(6) . 3\_645 ?  
 O4 Cu2 O2 84.2(5) 2\_456 . ?  
 O1 Cu2 O2 88.1(5) . . ?  
 O5 Cu2 O2 72.2(5) 4\_564 . ?  
 O4 Cu2 O2 91.7(5) . . ?  
 OW Cu2 O2 164.6(5) 3\_645 . ?  
 Te O1 Cu2 97.3(6) . . ?  
 Te O1 Cu1 90.8(5) . . ?  
 Cu2 O1 Cu1 91.1(5) . . ?  
 Te O1 OW 132.6(7) . . ?  
 Cu2 O1 OW 130.0(7) . . ?  
 Cu1 O1 OW 86.4(5) . . ?  
 Te O1 Pb 84.6(5) . 4\_664 ?  
 Cu2 O1 Pb 135.1(6) . 4\_664 ?  
 Cu1 O1 Pb 133.8(6) . 4\_664 ?  
 OW O1 Pb 64.7(5) . 4\_664 ?  
 Te O1 Cu1 73.3(4) . 2\_566 ?  
 Cu2 O1 Cu1 156.9(6) . 2\_566 ?  
 Cu1 O1 Cu1 68.5(3) . 2\_566 ?  
 OW O1 Cu1 61.7(4) . 2\_566 ?  
 Pb O1 Cu1 66.2(3) 4\_664 2\_566 ?  
 Te O1 Pb 174.2(7) . 4\_564 ?

Cu2 O1 Pb 84.5(4) . 4\_564 ?  
 Cu1 O1 Pb 83.6(4) . 4\_564 ?  
 OW O1 Pb 45.6(4) . 4\_564 ?  
 Pb O1 Pb 97.9(3) 4\_664 4\_564 ?  
 Cu1 O1 Pb 102.9(4) 2\_566 4\_564 ?  
 Te O1 Pb 60.4(3) . . ?  
 Cu2 O1 Pb 57.1(3) . . ?  
 Cu1 O1 Pb 53.3(3) . . ?  
 OW O1 Pb 139.6(6) . . ?  
 Pb O1 Pb 145.1(4) 4\_664 . ?  
 Cu1 O1 Pb 100.7(3) 2\_566 . ?  
 Pb O1 Pb 116.8(4) 4\_564 . ?  
 Te O2 Cu1 99.0(6) 1\_455 . ?  
 Te O2 Pb 160.9(7) 1\_455 . ?  
 Cu1 O2 Pb 100.1(6) . . ?  
 Te O2 Cu2 88.6(5) 1\_455 . ?  
 Cu1 O2 Cu2 88.5(5) . . ?  
 Pb O2 Cu2 90.8(5) . . ?  
 Te O2 Cu2 75.4(4) 1\_455 2\_456 ?  
 Cu1 O2 Cu2 163.0(6) . 2\_456 ?  
 Pb O2 Cu2 85.9(4) . 2\_456 ?  
 Cu2 O2 Cu2 75.4(3) . 2\_456 ?  
 Te O2 Pb 61.6(3) 1\_455 1\_455 ?  
 Cu1 O2 Pb 136.2(6) . 1\_455 ?  
 Pb O2 Pb 104.2(4) . 1\_455 ?  
 Cu2 O2 Pb 126.5(5) . 1\_455 ?  
 Cu2 O2 Pb 55.4(2) 2\_456 1\_455 ?  
 Te O3 Cu1 130.6(7) 2\_466 . ?  
 Te O3 Cu1 97.6(6) 2\_466 2\_566 ?  
 Cu1 O3 Cu1 124.8(7) . 2\_566 ?  
 Te O3 Pb 87.3(5) 2\_466 3\_656 ?  
 Cu1 O3 Pb 93.0(5) . 3\_656 ?  
 Cu1 O3 Pb 117.8(5) 2\_566 3\_656 ?  
 Te O3 Cu1 60.5(4) 2\_466 2\_466 ?  
 Cu1 O3 Cu1 71.0(4) . 2\_466 ?  
 Cu1 O3 Cu1 135.5(5) 2\_566 2\_466 ?  
 Pb O3 Cu1 100.5(4) 3\_656 2\_466 ?  
 Te O3 Cu2 57.2(3) 2\_466 2\_566 ?  
 Cu1 O3 Cu2 166.0(6) . 2\_566 ?  
 Cu1 O3 Cu2 58.0(3) 2\_566 2\_566 ?  
 Pb O3 Cu2 74.9(3) 3\_656 2\_566 ?  
 Cu1 O3 Cu2 117.6(4) 2\_466 2\_566 ?  
 Te O4 Cu2 125.6(7) . 2\_556 ?  
 Te O4 Cu2 96.5(6) . . ?  
 Cu2 O4 Cu2 134.5(7) 2\_556 . ?  
 Te O4 Pb 99.8(6) . . ?  
 Cu2 O4 Pb 95.7(5) 2\_556 . ?  
 Cu2 O4 Pb 92.6(5) . . ?  
 Te O4 Pb 100.2(5) . 2\_556 ?  
 Cu2 O4 Pb 71.0(4) 2\_556 2\_556 ?  
 Cu2 O4 Pb 86.9(5) . 2\_556 ?  
 Pb O4 Pb 159.9(5) . 2\_556 ?  
 Te O4 Cu1 58.3(4) . . ?  
 Cu2 O4 Cu1 154.9(6) 2\_556 . ?

Cu2 O4 Cu1 59.7(4) . . ?  
 Pb O4 Cu1 60.3(3) . . ?  
 Pb O4 Cu1 134.1(4) 2\_556 . ?  
 Te O4 Cu2 57.7(3) . 1\_655 ?  
 Cu2 O4 Cu2 74.4(4) 2\_556 1\_655 ?  
 Cu2 O4 Cu2 126.5(6) . 1\_655 ?  
 Pb O4 Cu2 134.2(5) . 1\_655 ?  
 Pb O4 Cu2 58.1(2) 2\_556 1\_655 ?  
 Cu1 O4 Cu2 115.9(4) . 1\_655 ?  
 Te O5 Cu2 107.0(6) 4\_665 4\_565 ?  
 Te O5 Pb 101.4(6) 4\_665 . ?  
 Cu2 O5 Pb 128.8(7) 4\_565 . ?  
 Te O5 Pb 118.2(6) 4\_665 3\_656 ?  
 Cu2 O5 Pb 84.3(5) 4\_565 3\_656 ?  
 Pb O5 Pb 117.9(5) . 3\_656 ?  
 Te O5 Cu1 61.4(4) 4\_665 4\_565 ?  
 Cu2 O5 Cu1 67.2(4) 4\_565 4\_565 ?  
 Pb O5 Cu1 91.8(4) . 4\_565 ?  
 Pb O5 Cu1 148.1(4) 3\_656 4\_565 ?  
 Te O5 Cu2 54.9(4) 4\_665 4\_665 ?  
 Cu2 O5 Cu2 133.2(6) 4\_565 4\_665 ?  
 Pb O5 Cu2 98.0(4) . 4\_665 ?  
 Pb O5 Cu2 73.0(3) 3\_656 4\_665 ?  
 Cu1 O5 Cu2 116.3(4) 4\_565 4\_665 ?  
 Te O5 Cu1 149.5(6) 4\_665 . ?  
 Cu2 O5 Cu1 103.3(5) 4\_565 . ?  
 Pb O5 Cu1 59.7(3) . . ?  
 Pb O5 Cu1 62.4(2) 3\_656 . ?  
 Cu1 O5 Cu1 136.0(4) 4\_565 . ?  
 Cu2 O5 Cu1 101.4(3) 4\_665 . ?  
 Te O5 Cu2 66.4(4) 4\_665 3\_656 ?  
 Cu2 O5 Cu2 72.7(4) 4\_565 3\_656 ?  
 Pb O5 Cu2 158.5(5) . 3\_656 ?  
 Pb O5 Cu2 59.7(2) 3\_656 3\_656 ?  
 Cu1 O5 Cu2 96.9(3) 4\_565 3\_656 ?  
 Cu2 O5 Cu2 60.5(2) 4\_665 3\_656 ?  
 Cu1 O5 Cu2 122.1(4) . 3\_656 ?  
 Te O6 Cu1 104.0(6) . . ?  
 Te O6 Pb 110.3(7) . . ?  
 Cu1 O6 Pb 96.8(6) . . ?  
 Te O6 Cu2 59.7(4) . . ?  
 Cu1 O6 Cu2 66.0(4) . . ?  
 Pb O6 Cu2 71.1(4) . . ?  
 Te O6 Cu1 73.2(4) . 2\_566 ?  
 Cu1 O6 Cu1 71.9(4) . 2\_566 ?  
 Pb O6 Cu1 168.8(6) . 2\_566 ?  
 Cu2 O6 Cu1 103.0(3) . 2\_566 ?  
 Te O6 Pb 145.2(6) . 3\_656 ?  
 Cu1 O6 Pb 72.7(4) . 3\_656 ?  
 Pb O6 Pb 104.5(4) . 3\_656 ?  
 Cu2 O6 Pb 137.3(4) . 3\_656 ?  
 Cu1 O6 Pb 73.0(3) 2\_566 3\_656 ?  
 Te O6 Cu1 51.9(3) . 1\_655 ?  
 Cu1 O6 Cu1 127.4(5) . 1\_655 ?

Pb O6 Cu1 133.7(5) . 1\_655 ?  
 Cu2 O6 Cu1 111.5(3) . 1\_655 ?  
 Cu1 O6 Cu1 57.1(2) 2\_566 1\_655 ?  
 Pb O6 Cu1 101.6(4) 3\_656 1\_655 ?  
 Te O6 Cu2 117.8(6) . 4\_665 ?  
 Cu1 O6 Cu2 133.6(6) . 4\_665 ?  
 Pb O6 Cu2 87.3(3) . 4\_665 ?  
 Cu2 O6 Cu2 153.7(4) . 4\_665 ?  
 Cu1 O6 Cu2 100.7(3) 2\_566 4\_665 ?  
 Pb O6 Cu2 61.7(2) 3\_656 4\_665 ?  
 Cu1 O6 Cu2 72.5(3) 1\_655 4\_665 ?  
 Te O6 OW 64.9(4) . . ?  
 Cu1 O6 OW 43.3(4) . . ?  
 Pb O6 OW 126.7(5) . . ?  
 Cu2 O6 OW 61.2(3) . . ?  
 Cu1 O6 OW 44.2(2) 2\_566 . ?  
 Pb O6 OW 95.4(3) 3\_656 . ?  
 Cu1 O6 OW 87.4(3) 1\_655 . ?  
 Cu2 O6 OW 144.3(4) 4\_665 . ?  
 Cu2 OW O1 139.7(7) 3\_655 . ?  
 Cu2 OW Pb 102.9(5) 3\_655 4\_564 ?  
 O1 OW Pb 89.3(5) . 4\_564 ?  
 Cu2 OW Pb 79.1(4) 3\_655 4\_664 ?  
 O1 OW Pb 63.4(5) . 4\_664 ?  
 Pb OW Pb 126.9(5) 4\_564 4\_664 ?  
 Cu2 OW Cu1 109.4(6) 3\_655 2\_566 ?  
 O1 OW Cu1 71.8(4) . 2\_566 ?  
 Pb OW Cu1 146.6(5) 4\_564 2\_566 ?  
 Pb OW Cu1 69.2(4) 4\_664 2\_566 ?  
 Cu2 OW Cu1 170.2(6) 3\_655 . ?  
 O1 OW Cu1 43.6(4) . . ?  
 Pb OW Cu1 85.7(4) 4\_564 . ?  
 Pb OW Cu1 99.5(4) 4\_664 . ?  
 Cu1 OW Cu1 61.4(2) 2\_566 . ?  
 Cu2 OW Cu1 125.0(5) 3\_655 2\_466 ?  
 O1 OW Cu1 94.8(5) . 2\_466 ?  
 Pb OW Cu1 62.3(3) 4\_564 2\_466 ?  
 Pb OW Cu1 153.9(4) 4\_664 2\_466 ?  
 Cu1 OW Cu1 91.4(3) 2\_566 2\_466 ?  
 Cu1 OW Cu1 54.9(2) . 2\_466 ?  
 Cu2 OW O6 152.3(7) 3\_655 . ?  
 O1 OW O6 30.3(4) . . ?  
 Pb OW O6 102.4(4) 4\_564 . ?  
 Pb OW O6 76.8(4) 4\_664 . ?  
 Cu1 OW O6 48.6(3) 2\_566 . ?  
 Cu1 OW O6 23.0(2) . . ?  
 Cu1 OW O6 77.3(3) 2\_466 . ?

\_diffn\_measured\_fraction\_theta\_max 0.998  
 \_diffn\_reflns\_theta\_full 24.70  
 \_diffn\_measured\_fraction\_theta\_full 0.998  
 \_refine\_diff\_density\_max 1.708  
 \_refine\_diff\_density\_min -2.210  
 \_refine\_diff\_density\_rms 0.417