

data_thorneite

_audit_creation_method SHELXL-97

_chemical_name_systematic

;

?

;

_chemical_name_common ?

_chemical_melting_point ?

_chemical_formula_moiety ?

_chemical_formula_sum

'C2 H5 Cl3 O29 Pb12 Te4'

_chemical_formula_weight 3596.09

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scat_dispersion_real

_atom_type_scat_dispersion_imag

_atom_type_scat_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'

'C' 'C' 0.0033 0.0016

'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

'Cl' 'Cl' 0.1484 0.1585

'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, y, -z+1/2'

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

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

'-x, -y, -z'

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

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

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

_cell_length_a 21.304(3)

_cell_length_b 11.0587(15)

_cell_length_c 7.5636(11)

_cell_angle_alpha 90.00

_cell_angle_beta 101.112(4)

_cell_angle_gamma 90.00
_cell_volume 1748.6(4)
_cell_formula_units_Z 2
_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 0.09
_exptl_crystal_size_mid 0.07
_exptl_crystal_size_min 0.02
_exptl_crystal_density_meas ?
_exptl_crystal_density_diffn 6.830
_exptl_crystal_density_method 'not measured'
_exptl_crystal_F_000 2984
_exptl_absorpt_coefficient_mu 61.129
_exptl_absorpt_correction_type ?
_exptl_absorpt_correction_T_min 0.0782
_exptl_absorpt_correction_T_max 0.4608
_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 8170
_diffrn_reflns_av_R_equivalents 0.0610
_diffrn_reflns_av_sigmaI/netI 0.0357
_diffrn_reflns_limit_h_min -23
_diffrn_reflns_limit_h_max 23
_diffrn_reflns_limit_k_min -12
_diffrn_reflns_limit_k_max 12
_diffrn_reflns_limit_l_min -7
_diffrn_reflns_limit_l_max 8
_diffrn_reflns_theta_min 3.46
_diffrn_reflns_theta_max 23.24
_reflns_number_total 1255
_reflns_number_gt 1135
_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 > 2sigma(F^2) is used only for calculating R-factors(gt) etc. and is
not relevant to the choice of reflections for refinement. R-factors based
on F^2 are statistically about twice as large as those based on F, and R-
factors based on ALL data will be even larger.
;

_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+107.0748P] where P=(Fo^2+2Fc^2)/3'
_atom_sites_solution_primary    direct
_atom_sites_solution_secondary  difmap
_atom_sites_solution_hydrogens  geom
_refine_lsHydrogen_treatment   mixed
_refine_ls_extinction_method   none
_refine_ls_extinction_coef     ?
_refine_ls_number_reflns       1255
_refine_ls_number_parameters   120
_refine_ls_number_restraints   2
_refine_ls_R_factor_all        0.0331
_refine_ls_R_factor_gt         0.0283
_refine_ls_wR_factor_ref       0.0553
_refine_ls_wR_factor_gt        0.0537
_refine_ls_goodness_of_fit_ref 1.069
_refine_ls_restrained_S_all   1.068
_refine_ls_shift/su_max        0.001
_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
Pb1 Pb 0.63753(3) 0.09635(5) 0.15303(7) 0.01863(17) Uani 1 1 d ...
Pb2 Pb 0.69515(3) 0.41296(5) 0.96922(8) 0.02200(18) Uani 1 1 d ...
Pb3 Pb 0.55264(3) 0.24366(6) 0.52254(8) 0.02826(19) Uani 1 1 d ...
Te Te 0.78842(5) 0.30010(8) 0.36271(12) 0.0134(2) Uani 1 1 d ...
C C 0.5000 -0.018(2) 0.2500 0.025(6) Uani 1 2 d S ..
Cl Cl 0.5884(3) 0.3933(6) 0.1682(8) 0.057(3) Uani 0.75(4) 1 d P ..
OH O 0.5884(3) 0.3933(6) 0.1682(8) 0.057(3) Uani 0.25(4) 1 d P ..
O1 O 0.5000 0.0990(15) 0.2500 0.053(5) Uani 1 2 d S ..
O2 O 0.5487(6) 0.9266(11) 0.2183(17) 0.044(3) Uani 1 1 d ...
O3 O 0.7815(5) 0.4526(9) 0.2479(13) 0.026(3) Uani 1 1 d ...
O4 O 0.6451(5) 0.2717(9) 0.7367(12) 0.020(2) Uani 1 1 d ...
O5 O 0.7269(5) 0.2338(8) 0.1654(12) 0.016(2) Uani 1 1 d ...
O6 O 0.6435(4) 0.1381(8) 0.4534(12) 0.014(2) Uani 1 1 d ...
O7 O 0.7201(4) 0.3460(8) 0.4937(12) 0.012(2) Uani 1 1 d ...
OW O 0.5000 0.391(2) 0.7500 0.089(8) Uani 1 2 d SD ..
H H 0.525(8) 0.442(5) 0.829(19) 0.08(8) Uiso 1 1 d 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
Pb1 0.0139(3) 0.0242(3) 0.0165(3) -0.0012(2) -0.0005(2) 0.0015(3)
Pb2 0.0218(4) 0.0233(3) 0.0195(3) -0.0021(3) 0.0007(3) -0.0020(3)
Pb3 0.0177(4) 0.0376(4) 0.0279(4) -0.0047(3) 0.0006(3) 0.0056(3)
Te 0.0114(5) 0.0160(5) 0.0128(5) -0.0008(4) 0.0024(4) -0.0030(4)
C 0.028(16) 0.016(13) 0.025(13) 0.000 -0.010(11) 0.000
Cl 0.032(4) 0.080(6) 0.059(5) -0.002(3) 0.009(3) 0.006(3)
OH 0.032(4) 0.080(6) 0.059(5) -0.002(3) 0.009(3) 0.006(3)
O1 0.034(12) 0.033(11) 0.079(14) 0.000 -0.015(10) 0.000
O2 0.022(7) 0.049(8) 0.063(9) -0.009(7) 0.013(6) 0.001(6)
O3 0.024(7) 0.028(6) 0.021(6) 0.008(5) -0.006(5) -0.011(5)
O4 0.016(6) 0.028(6) 0.016(5) -0.012(5) 0.003(5) -0.008(5)
O5 0.013(6) 0.019(6) 0.014(5) 0.004(4) -0.004(4) -0.004(4)
O6 0.008(5) 0.025(6) 0.010(5) -0.002(4) 0.003(4) -0.001(4)
O7 0.011(6) 0.013(5) 0.014(5) -0.003(4) 0.008(4) 0.002(4)
OW 0.09(2) 0.09(2) 0.08(2) 0.000 0.022(17) 0.000

_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
Pb1 O6 2.297(9) . ?
Pb1 O3 2.360(10) 4_645 ?
Pb1 O5 2.423(9) . ?
Pb1 O2 2.777(12) 1_545 ?
Pb1 O6 3.016(9) 6 ?
Pb1 O1 3.1548(7) . ?
Pb1 C 3.398(8) . ?
Pb1 Cl 3.456(7) . ?
Pb1 O2 3.472(13) 6_565 ?
Pb1 Te 3.6481(11) 4_645 ?
Pb1 O7 3.692(9) 7_656 ?
Pb1 O4 3.728(10) 1_554 ?
Pb1 O3 3.806(10) 7_655 ?
Pb1 Pb2 3.8525(10) 7_656 ?
Pb2 O4 2.439(9) . ?
Pb2 O5 2.490(9) 1_556 ?
Pb2 O3 2.554(10) 1_556 ?
Pb2 O5 2.661(9) 7_656 ?
Pb2 O7 2.718(9) 6_566 ?
Pb2 OH 2.968(6) 1_556 ?
Pb2 Cl 2.968(6) 1_556 ?
Pb2 O3 3.096(11) 6_566 ?
Pb2 Te 3.4763(12) 1_556 ?
Pb2 Te 3.5093(11) 7_656 ?
Pb2 OH 3.599(7) 6_566 ?
Pb2 Cl 3.599(7) 6_566 ?
Pb2 O7 3.808(8) . ?
Pb2 Pb1 3.8526(10) 7_656 ?
Pb2 Te 3.9095(12) 6_566 ?
Pb3 O4 2.317(10) . ?
Pb3 O6 2.404(9) . ?
Pb3 O2 2.406(12) 6_566 ?
Pb3 O1 2.679(10) . ?
Pb3 OW 2.758(16) . ?
Pb3 C 3.347(16) 5_656 ?
Pb3 Cl 3.360(6) . ?
Pb3 Te 3.3646(13) 7_656 ?
Pb3 OH 3.489(7) 2_655 ?
Pb3 Cl 3.489(7) 2_655 ?
Pb3 C 3.602(18) . ?
Pb3 O2 3.699(12) 5_666 ?
Pb3 O7 3.788(9) . ?
Te O3 1.889(10) . ?
Te O4 1.901(9) 7_656 ?
Te O6 1.930(9) 7_656 ?
Te O5 1.931(9) . ?
Te O7 1.974(9) 7_656 ?
Te O7 1.979(8) . ?

Te Te 3.0872(18) 7_656 ?
Te Pb3 3.3647(13) 7_656 ?
Te Pb2 3.4762(12) 1_554 ?
Te Pb2 3.5093(11) 7_656 ?
Te Pb1 3.6481(11) 4_655 ?
Te Pb1 3.8715(12) 7_656 ?
C O2 1.269(15) 2_645 ?
C O2 1.269(15) 1_545 ?
C O1 1.29(3) . ?
C Pb3 3.346(16) 5_656 ?
C Pb3 3.346(16) 6 ?
C Pb1 3.398(8) 2_655 ?
C Pb3 3.602(17) 2_655 ?
C Pb1 3.897(5) 6_556 ?
C Pb1 3.897(5) 5_655 ?
Cl Pb2 2.968(6) 1_554 ?
Cl Pb3 3.489(7) 2_655 ?
Cl Pb2 3.599(7) 6_565 ?
Cl Pb3 4.194(7) 6_565 ?
Cl OW 5.109(6) . ?
Cl H 5.4(2) . ?
O1 Pb3 2.679(10) 2_655 ?
O1 Pb1 3.1548(7) 2_655 ?
O2 C 1.269(15) 1_565 ?
O2 Pb3 2.406(12) 6_565 ?
O2 Pb1 2.777(12) 1_565 ?
O2 Pb1 3.472(13) 6_566 ?
O2 Pb3 3.699(12) 5_666 ?
O3 Pb1 2.360(10) 4_655 ?
O3 Pb2 2.554(10) 1_554 ?
O3 Pb2 3.095(11) 6_565 ?
O3 Pb1 3.806(10) 7_655 ?
O4 Te 1.901(9) 7_656 ?
O4 Pb1 3.728(10) 1_556 ?
O4 Pb1 4.118(10) 6_556 ?
O5 Pb2 2.490(9) 1_554 ?
O5 Pb2 2.661(9) 7_656 ?
O6 Te 1.930(9) 7_656 ?
O6 Pb1 3.016(9) 6_556 ?
O7 Te 1.974(9) 7_656 ?
O7 Pb2 2.718(9) 6_565 ?
O7 Pb1 3.692(9) 7_656 ?
O7 Pb2 3.969(9) 1_554 ?
OW H 0.92(3) . ?
OW Pb3 2.758(16) 2_656 ?
OW H 0.92(3) . ?

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
O6 Pb1 O3 85.6(3) . 4_645 ?
O6 Pb1 O5 86.7(3) . . ?
O3 Pb1 O5 83.7(3) 4_645 . ?
O6 Pb1 O2 82.5(3) . 1_545 ?
O3 Pb1 O2 88.2(4) 4_645 1_545 ?
O5 Pb1 O2 167.0(4) . 1_545 ?
O6 Pb1 O6 131.9(2) . 6 ?
O3 Pb1 O6 58.7(3) 4_645 6 ?
O5 Pb1 O6 116.7(3) . 6 ?
O2 Pb1 O6 66.7(3) 1_545 6 ?
O6 Pb1 O1 69.2(2) . . ?
O3 Pb1 O1 126.0(4) 4_645 . ?
O5 Pb1 O1 138.0(4) . . ?
O2 Pb1 O1 43.1(4) 1_545 . ?
O6 Pb1 O1 104.8(3) 6 . ?
O6 Pb1 C 75.4(3) . . ?
O3 Pb1 C 106.8(4) 4_645 . ?
O5 Pb1 C 158.2(4) . . ?
O2 Pb1 C 20.7(4) 1_545 . ?
O6 Pb1 C 84.8(3) 6 . ?
O1 Pb1 C 22.3(4) . . ?
O6 Pb1 Cl 74.7(3) . . ?
O3 Pb1 Cl 146.9(3) 4_645 . ?
O5 Pb1 Cl 69.1(2) . . ?
O2 Pb1 Cl 114.6(3) 1_545 . ?
O6 Pb1 Cl 151.2(2) 6 . ?
O1 Pb1 Cl 71.5(3) . . ?
C Pb1 Cl 93.8(4) . . ?
O6 Pb1 O2 150.1(3) . 6_565 ?
O3 Pb1 O2 118.9(3) 4_645 6_565 ?
O5 Pb1 O2 111.3(3) . 6_565 ?
O2 Pb1 O2 81.6(3) 1_545 6_565 ?
O6 Pb1 O2 62.0(3) 6 6_565 ?
O1 Pb1 O2 81.94(19) . 6_565 ?
C Pb1 O2 80.92(19) . 6_565 ?
Cl Pb1 O2 89.3(2) . 6_565 ?
O6 Pb1 Te 105.7(2) . 4_645 ?
O3 Pb1 Te 27.2(2) 4_645 4_645 ?
O5 Pb1 Te 102.9(2) . 4_645 ?
O2 Pb1 Te 73.3(3) 1_545 4_645 ?
O6 Pb1 Te 31.91(18) 6 4_645 ?
O1 Pb1 Te 116.3(3) . 4_645 ?
C Pb1 Te 94.0(3) . 4_645 ?
Cl Pb1 Te 172.00(11) . 4_645 ?
O2 Pb1 Te 93.7(2) 6_565 4_645 ?
O6 Pb1 O7 50.8(3) . 7_656 ?
O3 Pb1 O7 55.8(3) 4_645 7_656 ?
O5 Pb1 O7 48.2(3) . 7_656 ?
O2 Pb1 O7 118.8(3) 1_545 7_656 ?
O6 Pb1 O7 113.8(2) 6 7_656 ?
O1 Pb1 O7 120.05(14) . 7_656 ?
C Pb1 O7 122.04(13) . 7_656 ?
Cl Pb1 O7 91.36(17) . 7_656 ?

O2 Pb1 O7 156.9(2) 6_565 7_656 ?
Te Pb1 O7 83.03(13) 4_645 7_656 ?
O6 Pb1 O4 136.7(3) . 1_554 ?
O3 Pb1 O4 118.1(3) 4_645 1_554 ?
O5 Pb1 O4 62.9(3) . 1_554 ?
O2 Pb1 O4 130.1(3) 1_545 1_554 ?
O6 Pb1 O4 90.7(2) 6 1_554 ?
O1 Pb1 O4 112.6(2) . 1_554 ?
C Pb1 O4 123.7(2) . 1_554 ?
Cl Pb1 O4 66.20(18) . 1_554 ?
O2 Pb1 O4 48.9(2) 6_565 1_554 ?
Te Pb1 O4 110.50(15) 4_645 1_554 ?
O7 Pb1 O4 111.0(2) 7_656 1_554 ?
O6 Pb1 O3 150.4(3) . 7_655 ?
O3 Pb1 O3 75.0(3) 4_645 7_655 ?
O5 Pb1 O3 69.3(3) . 7_655 ?
O2 Pb1 O3 118.3(3) 1_545 7_655 ?
O6 Pb1 O3 53.8(2) 6 7_655 ?
O1 Pb1 O3 140.41(17) . 7_655 ?
C Pb1 O3 131.4(2) . 7_655 ?
Cl Pb1 O3 110.39(18) . 7_655 ?
O2 Pb1 O3 58.9(2) 6_565 7_655 ?
Te Pb1 O3 65.23(15) 4_645 7_655 ?
O7 Pb1 O3 99.5(2) 7_656 7_655 ?
O4 Pb1 O3 45.6(2) 1_554 7_655 ?
O6 Pb1 Pb2 111.4(2) . 7_656 ?
O3 Pb1 Pb2 53.4(3) 4_645 7_656 ?
O5 Pb1 Pb2 43.1(2) . 7_656 ?
O2 Pb1 Pb2 135.9(3) 1_545 7_656 ?
O6 Pb1 Pb2 74.12(17) 6 7_656 ?
O1 Pb1 Pb2 178.9(3) . 7_656 ?
C Pb1 Pb2 156.7(3) . 7_656 ?
Cl Pb1 Pb2 109.49(10) . 7_656 ?
O2 Pb1 Pb2 97.55(19) 6_565 7_656 ?
Te Pb1 Pb2 62.76(2) 4_645 7_656 ?
O7 Pb1 Pb2 60.59(13) 7_656 7_656 ?
O4 Pb1 Pb2 67.58(15) 1_554 7_656 ?
O3 Pb1 Pb2 38.96(16) 7_655 7_656 ?
O4 Pb2 O5 87.2(3) . 1_556 ?
O4 Pb2 O3 148.2(3) . 1_556 ?
O5 Pb2 O3 64.9(3) 1_556 1_556 ?
O4 Pb2 O5 63.4(3) . 7_656 ?
O5 Pb2 O5 68.0(3) 1_556 7_656 ?
O3 Pb2 O5 91.0(3) 1_556 7_656 ?
O4 Pb2 O7 136.9(3) . 6_566 ?
O5 Pb2 O7 135.5(3) 1_556 6_566 ?
O3 Pb2 O7 71.1(3) 1_556 6_566 ?
O5 Pb2 O7 119.7(3) 7_656 6_566 ?
O4 Pb2 OH 92.7(3) . 1_556 ?
O5 Pb2 OH 77.6(3) 1_556 1_556 ?
O3 Pb2 OH 95.4(3) 1_556 1_556 ?
O5 Pb2 OH 138.2(2) 7_656 1_556 ?
O7 Pb2 OH 101.3(2) 6_566 1_556 ?
O4 Pb2 Cl 92.7(3) . 1_556 ?

O5 Pb2 Cl 77.6(3) 1_556 1_556 ?
O3 Pb2 Cl 95.4(3) 1_556 1_556 ?
O5 Pb2 Cl 138.2(2) 7_656 1_556 ?
O7 Pb2 Cl 101.3(2) 6_566 1_556 ?
OH Pb2 Cl 0.0(3) 1_556 1_556 ?
O4 Pb2 O3 98.1(3) . 6_566 ?
O5 Pb2 O3 125.7(3) 1_556 6_566 ?
O3 Pb2 O3 87.4(3) 1_556 6_566 ?
O5 Pb2 O3 66.8(3) 7_656 6_566 ?
O7 Pb2 O3 55.7(2) 6_566 6_566 ?
OH Pb2 O3 154.5(2) 1_556 6_566 ?
Cl Pb2 O3 154.5(2) 1_556 6_566 ?
O4 Pb2 Te 119.1(2) . 1_556 ?
O5 Pb2 Te 32.8(2) 1_556 1_556 ?
O3 Pb2 Te 32.1(2) 1_556 1_556 ?
O5 Pb2 Te 79.2(2) 7_656 1_556 ?
O7 Pb2 Te 102.8(2) 6_566 1_556 ?
OH Pb2 Te 84.67(13) 1_556 1_556 ?
Cl Pb2 Te 84.67(13) 1_556 1_556 ?
O3 Pb2 Te 109.53(19) 6_566 1_556 ?
O4 Pb2 Te 31.1(2) . 7_656 ?
O5 Pb2 Te 80.7(2) 1_556 7_656 ?
O3 Pb2 Te 123.4(2) 1_556 7_656 ?
O5 Pb2 Te 33.0(2) 7_656 7_656 ?
O7 Pb2 Te 131.47(18) 6_566 7_656 ?
OH Pb2 Te 120.37(13) 1_556 7_656 ?
Cl Pb2 Te 120.37(13) 1_556 7_656 ?
O3 Pb2 Te 77.53(18) 6_566 7_656 ?
Te Pb2 Te 104.60(3) 1_556 7_656 ?
O4 Pb2 OH 77.9(3) . 6_566 ?
O5 Pb2 OH 156.5(2) 1_556 6_566 ?
O3 Pb2 OH 133.4(3) 1_556 6_566 ?
O5 Pb2 OH 119.1(2) 7_656 6_566 ?
O7 Pb2 OH 63.3(2) 6_566 6_566 ?
OH Pb2 OH 84.93(16) 1_556 6_566 ?
Cl Pb2 OH 84.93(16) 1_556 6_566 ?
O3 Pb2 OH 75.0(2) 6_566 6_566 ?
Te Pb2 OH 160.51(11) 1_556 6_566 ?
Te Pb2 OH 94.88(11) 7_656 6_566 ?
O4 Pb2 Cl 77.9(3) . 6_566 ?
O5 Pb2 Cl 156.5(2) 1_556 6_566 ?
O3 Pb2 Cl 133.4(3) 1_556 6_566 ?
O5 Pb2 Cl 119.1(2) 7_656 6_566 ?
O7 Pb2 Cl 63.3(2) 6_566 6_566 ?
OH Pb2 Cl 84.93(16) 1_556 6_566 ?
Cl Pb2 Cl 84.93(16) 1_556 6_566 ?
O3 Pb2 Cl 75.0(2) 6_566 6_566 ?
Te Pb2 Cl 160.51(11) 1_556 6_566 ?
Te Pb2 Cl 94.88(11) 7_656 6_566 ?
OH Pb2 Cl 0.0(2) 6_566 6_566 ?
O4 Pb2 O7 46.8(3) . . ?
O5 Pb2 O7 109.7(3) 1_556 . ?
O3 Pb2 O7 127.1(3) 1_556 . ?
O5 Pb2 O7 46.3(2) 7_656 . ?

O7 Pb2 O7 101.2(2) 6_566 . ?
OH Pb2 O7 136.45(19) 1_556 . ?
Cl Pb2 O7 136.45(19) 1_556 . ?
O3 Pb2 O7 51.5(2) 6_566 . ?
Te Pb2 O7 125.31(14) 1_556 . ?
Te Pb2 O7 30.96(13) 7_656 . ?
OH Pb2 O7 72.81(17) 6_566 . ?
Cl Pb2 O7 72.81(17) 6_566 . ?
O4 Pb2 Pb1 96.1(2) . 7_656 ?
O5 Pb2 Pb1 88.0(2) 1_556 7_656 ?
O3 Pb2 Pb1 69.5(2) 1_556 7_656 ?
O5 Pb2 Pb1 38.5(2) 7_656 7_656 ?
O7 Pb2 Pb1 82.24(18) 6_566 7_656 ?
OH Pb2 Pb1 162.72(13) 1_556 7_656 ?
Cl Pb2 Pb1 162.72(13) 1_556 7_656 ?
O3 Pb2 Pb1 37.76(19) 6_566 7_656 ?
Te Pb2 Pb1 78.07(2) 1_556 7_656 ?
Te Pb2 Pb1 65.54(2) 7_656 7_656 ?
OH Pb2 Pb1 111.43(10) 6_566 7_656 ?
Cl Pb2 Pb1 111.43(10) 6_566 7_656 ?
O7 Pb2 Pb1 57.61(14) . 7_656 ?
O4 Pb2 Te 122.7(2) . 6_566 ?
O5 Pb2 Te 132.7(2) 1_556 6_566 ?
O3 Pb2 Te 73.6(2) 1_556 6_566 ?
O5 Pb2 Te 92.1(2) 7_656 6_566 ?
O7 Pb2 Te 28.05(18) 6_566 6_566 ?
OH Pb2 Te 129.32(13) 1_556 6_566 ?
Cl Pb2 Te 129.32(13) 1_556 6_566 ?
O3 Pb2 Te 28.37(18) 6_566 6_566 ?
Te Pb2 Te 103.80(3) 1_556 6_566 ?
Te Pb2 Te 105.831(18) 7_656 6_566 ?
OH Pb2 Te 70.78(10) 6_566 6_566 ?
Cl Pb2 Te 70.78(10) 6_566 6_566 ?
O7 Pb2 Te 78.14(13) . 6_566 ?
Pb1 Pb2 Te 56.061(19) 7_656 6_566 ?
O4 Pb3 O6 66.7(3) . . ?
O4 Pb3 O2 78.5(4) . 6_566 ?
O6 Pb3 O2 83.0(4) . 6_566 ?
O4 Pb3 O1 142.3(3) . . ?
O6 Pb3 O1 77.2(3) . . ?
O2 Pb3 O1 87.0(4) 6_566 . ?
O4 Pb3 OW 83.0(2) . . ?
O6 Pb3 OW 149.7(2) . . ?
O2 Pb3 OW 90.6(5) 6_566 . ?
O1 Pb3 OW 132.22(18) . . ?
O4 Pb3 C 93.7(2) . 5_656 ?
O6 Pb3 C 96.5(3) . 5_656 ?
O2 Pb3 C 17.3(3) 6_566 5_656 ?
O1 Pb3 C 79.5(3) . 5_656 ?
OW Pb3 C 84.4(5) . 5_656 ?
O4 Pb3 Cl 101.5(3) . . ?
O6 Pb3 Cl 75.5(2) . . ?
O2 Pb3 Cl 156.4(3) 6_566 . ?
O1 Pb3 Cl 78.8(3) . . ?

OW Pb3 Cl 112.9(4) . . ?
C Pb3 Cl 158.1(2) 5_656 . ?
O4 Pb3 Te 33.0(2) . 7_656 ?
O6 Pb3 Te 34.2(2) . 7_656 ?
O2 Pb3 Te 83.2(3) 6_566 7_656 ?
O1 Pb3 Te 111.33(14) . 7_656 ?
OW Pb3 Te 115.72(7) . 7_656 ?
C Pb3 Te 100.39(11) 5_656 7_656 ?
Cl Pb3 Te 84.55(11) . 7_656 ?
O4 Pb3 OH 140.7(3) . 2_655 ?
O6 Pb3 OH 143.7(2) . 2_655 ?
O2 Pb3 OH 119.8(3) 6_566 2_655 ?
O1 Pb3 OH 76.5(3) . 2_655 ?
OW Pb3 OH 63.71(17) . 2_655 ?
C Pb3 OH 102.68(16) 5_656 2_655 ?
Cl Pb3 OH 75.28(18) . 2_655 ?
Te Pb3 OH 156.69(11) 7_656 2_655 ?
O4 Pb3 Cl 140.7(3) . 2_655 ?
O6 Pb3 Cl 143.7(2) . 2_655 ?
O2 Pb3 Cl 119.8(3) 6_566 2_655 ?
O1 Pb3 Cl 76.5(3) . 2_655 ?
OW Pb3 Cl 63.71(17) . 2_655 ?
C Pb3 Cl 102.68(16) 5_656 2_655 ?
Cl Pb3 Cl 75.28(18) . 2_655 ?
Te Pb3 Cl 156.69(11) 7_656 2_655 ?
OH Pb3 Cl 0.00(13) 2_655 2_655 ?
O4 Pb3 C 129.5(3) . . ?
O6 Pb3 C 70.2(2) . . ?
O2 Pb3 C 71.4(4) 6_566 . ?
O1 Pb3 C 16.7(3) . . ?
OW Pb3 C 135.3(3) . . ?
C Pb3 C 66.23(5) 5_656 . ?
Cl Pb3 C 91.9(2) . . ?
Te Pb3 C 102.65(12) 7_656 . ?
OH Pb3 C 89.8(2) 2_655 . ?
Cl Pb3 C 89.8(2) 2_655 . ?
O4 Pb3 O2 101.7(3) . 5_666 ?
O6 Pb3 O2 116.4(3) . 5_666 ?
O2 Pb3 O2 35.2(4) 6_566 5_666 ?
O1 Pb3 O2 84.4(3) . 5_666 ?
OW Pb3 O2 67.7(5) . 5_666 ?
C Pb3 O2 19.9(3) 5_656 5_666 ?
Cl Pb3 O2 156.7(2) . 5_666 ?
Te Pb3 O2 116.8(2) 7_656 5_666 ?
OH Pb3 O2 85.2(2) 2_655 5_666 ?
Cl Pb3 O2 85.2(2) 2_655 5_666 ?
C Pb3 O2 75.3(2) . 5_666 ?
O4 Pb3 O7 47.0(3) . . ?
O6 Pb3 O7 47.6(3) . . ?
O2 Pb3 O7 114.4(3) 6_566 . ?
O1 Pb3 O7 113.15(13) . . ?
OW Pb3 O7 111.1(3) . . ?
C Pb3 O7 131.69(17) 5_656 . ?
Cl Pb3 O7 56.37(18) . . ?

Te Pb3 O7 31.33(14) 7_656 . ?
OH Pb3 O7 125.43(17) 2_655 . ?
Cl Pb3 O7 125.43(17) 2_655 . ?
C Pb3 O7 113.54(13) . . ?
O2 Pb3 O7 146.6(2) 5_666 . ?
O4 Pb3 Pb1 96.1(2) . . ?
O6 Pb3 Pb1 31.8(2) . . ?
O2 Pb3 Pb1 100.8(3) 6_566 . ?
O1 Pb3 Pb1 52.53(3) . . ?
OW Pb3 Pb1 168.1(4) . . ?
C Pb3 Pb1 107.4(2) 5_656 . ?
Cl Pb3 Pb1 55.61(11) . . ?
Te Pb3 Pb1 63.20(2) 7_656 . ?
OH Pb3 Pb1 112.16(10) 2_655 . ?
Cl Pb3 Pb1 112.16(10) 2_655 . ?
C Pb3 Pb1 53.14(3) . . ?
O2 Pb3 Pb1 123.87(19) 5_666 . ?
O7 Pb3 Pb1 61.25(13) . . ?
O3 Te O4 100.9(4) . 7_656 ?
O3 Te O6 89.8(4) . 7_656 ?
O4 Te O6 85.4(4) 7_656 7_656 ?
O3 Te O5 90.1(4) . . ?
O4 Te O5 89.0(4) 7_656 . ?
O6 Te O5 174.3(4) 7_656 . ?
O3 Te O7 167.4(4) . 7_656 ?
O4 Te O7 91.7(4) 7_656 7_656 ?
O6 Te O7 91.6(4) 7_656 7_656 ?
O5 Te O7 89.7(4) . 7_656 ?
O3 Te O7 90.1(4) . . ?
O4 Te O7 169.0(4) 7_656 . ?
O6 Te O7 94.1(4) 7_656 . ?
O5 Te O7 91.6(4) . . ?
O7 Te O7 77.3(4) 7_656 . ?
O3 Te Te 128.7(3) . 7_656 ?
O4 Te Te 130.4(3) 7_656 7_656 ?
O6 Te Te 93.7(3) 7_656 7_656 ?
O5 Te Te 90.8(3) . 7_656 ?
O7 Te Te 38.7(2) 7_656 7_656 ?
O7 Te Te 38.6(3) . 7_656 ?
O3 Te Pb3 103.5(3) . 7_656 ?
O4 Te Pb3 41.6(3) 7_656 7_656 ?
O6 Te Pb3 44.5(3) 7_656 7_656 ?
O5 Te Pb3 130.1(3) . 7_656 ?
O7 Te Pb3 86.2(3) 7_656 7_656 ?
O7 Te Pb3 135.2(3) . 7_656 ?
Te Te Pb3 114.37(5) 7_656 7_656 ?
O3 Te Pb2 46.0(3) . 1_554 ?
O4 Te Pb2 99.1(3) 7_656 1_554 ?
O6 Te Pb2 135.7(3) 7_656 1_554 ?
O5 Te Pb2 44.3(3) . 1_554 ?
O7 Te Pb2 131.8(3) 7_656 1_554 ?
O7 Te Pb2 89.0(3) . 1_554 ?
Te Te Pb2 114.53(5) 7_656 1_554 ?
Pb3 Te Pb2 130.79(3) 7_656 1_554 ?

O3 Te Pb2 106.3(3) . 7_656 ?
O4 Te Pb2 41.6(3) 7_656 7_656 ?
O6 Te Pb2 126.1(3) 7_656 7_656 ?
O5 Te Pb2 48.6(3) . 7_656 ?
O7 Te Pb2 82.9(2) 7_656 7_656 ?
O7 Te Pb2 135.6(3) . 7_656 ?
Te Te Pb2 112.29(4) 7_656 7_656 ?
Pb3 Te Pb2 81.59(2) 7_656 7_656 ?
Pb2 Te Pb2 75.40(3) 1_554 7_656 ?
O3 Te Pb1 34.9(3) . 4_655 ?
O4 Te Pb1 90.1(3) 7_656 4_655 ?
O6 Te Pb1 55.7(3) 7_656 4_655 ?
O5 Te Pb1 123.3(3) . 4_655 ?
O7 Te Pb1 147.0(3) 7_656 4_655 ?
O7 Te Pb1 98.7(3) . 4_655 ?
Te Te Pb1 129.27(4) 7_656 4_655 ?
Pb3 Te Pb1 73.59(2) 7_656 4_655 ?
Pb2 Te Pb1 80.16(2) 1_554 4_655 ?
Pb2 Te Pb1 118.44(3) 7_656 4_655 ?
O3 Te Pb1 98.8(3) . 7_656 ?
O4 Te Pb1 107.4(3) 7_656 7_656 ?
O6 Te Pb1 26.0(2) 7_656 7_656 ?
O5 Te Pb1 159.3(3) . 7_656 ?
O7 Te Pb1 77.6(3) 7_656 7_656 ?
O7 Te Pb1 69.9(3) . 7_656 ?
Te Te Pb1 69.02(3) 7_656 7_656 ?
Pb3 Te Pb1 65.93(2) 7_656 7_656 ?
Pb2 Te Pb1 139.93(3) 1_554 7_656 ?
Pb2 Te Pb1 142.82(3) 7_656 7_656 ?
Pb1 Te Pb1 70.45(2) 4_655 7_656 ?
O2 C O2 122(2) 2_645 1_545 ?
O2 C O1 119.0(11) 2_645 . ?
O2 C O1 119.0(11) 1_545 . ?
O2 C Pb3 34.3(8) 2_645 5_656 ?
O2 C Pb3 95.9(12) 1_545 5_656 ?
O1 C Pb3 138.3(2) . 5_656 ?
O2 C Pb3 95.9(12) 2_645 6 ?
O2 C Pb3 34.3(8) 1_545 6 ?
O1 C Pb3 138.3(2) . 6 ?
Pb3 C Pb3 83.5(5) 5_656 6 ?
O2 C Pb1 172.8(13) 2_645 . ?
O2 C Pb1 50.8(8) 1_545 . ?
O1 C Pb1 68.2(3) . . ?
Pb3 C Pb1 141.0(4) 5_656 . ?
Pb3 C Pb1 77.17(11) 6 . ?
O2 C Pb1 50.8(8) 2_645 2_655 ?
O2 C Pb1 172.8(13) 1_545 2_655 ?
O1 C Pb1 68.2(3) . 2_655 ?
Pb3 C Pb1 77.17(11) 5_656 2_655 ?
Pb3 C Pb1 141.0(4) 6 2_655 ?
Pb1 C Pb1 136.4(7) . 2_655 ?
O2 C Pb3 108.8(8) 2_645 2_655 ?
O2 C Pb3 117.2(8) 1_545 2_655 ?
O1 C Pb3 36.6(2) . 2_655 ?

Pb3 C Pb3 142.66(7) 5_656 2_655 ?
Pb3 C Pb3 113.77(5) 6 2_655 ?
Pb1 C Pb3 76.4(3) . 2_655 ?
Pb1 C Pb3 68.8(3) 2_655 2_655 ?
O2 C Pb3 117.2(8) 2_645 . ?
O2 C Pb3 108.8(8) 1_545 . ?
O1 C Pb3 36.6(2) . . ?
Pb3 C Pb3 113.77(5) 5_656 . ?
Pb3 C Pb3 142.66(7) 6 . ?
Pb1 C Pb3 68.8(3) . . ?
Pb1 C Pb3 76.4(3) 2_655 . ?
Pb3 C Pb3 73.2(4) 2_655 . ?
O2 C Pb1 105.3(8) 2_645 6_556 ?
O2 C Pb1 61.3(6) 1_545 6_556 ?
O1 C Pb1 102.9(3) . 6_556 ?
Pb3 C Pb1 73.0(2) 5_656 6_556 ?
Pb3 C Pb1 87.7(3) 6 6_556 ?
Pb1 C Pb1 72.66(2) . 6_556 ?
Pb1 C Pb1 117.62(8) 2_655 6_556 ?
Pb3 C Pb1 136.9(5) 2_655 6_556 ?
Pb3 C Pb1 68.11(11) . 6_556 ?
O2 C Pb1 61.3(6) 2_645 5_655 ?
O2 C Pb1 105.3(8) 1_545 5_655 ?
O1 C Pb1 102.9(3) . 5_655 ?
Pb3 C Pb1 87.7(3) 5_656 5_655 ?
Pb3 C Pb1 73.0(2) 6 5_655 ?
Pb1 C Pb1 117.62(8) . 5_655 ?
Pb1 C Pb1 72.66(3) 2_655 5_655 ?
Pb3 C Pb1 68.11(11) 2_655 5_655 ?
Pb3 C Pb1 136.9(5) . 5_655 ?
Pb1 C Pb1 154.2(6) 6_556 5_655 ?
Pb2 Cl Pb3 139.0(2) 1_554 . ?
Pb2 Cl Pb1 77.63(14) 1_554 . ?
Pb3 Cl Pb1 71.04(13) . . ?
Pb2 Cl Pb3 120.5(2) 1_554 2_655 ?
Pb3 Cl Pb3 77.69(14) . 2_655 ?
Pb1 Cl Pb3 77.16(14) . 2_655 ?
Pb2 Cl Pb2 79.89(15) 1_554 6_565 ?
Pb3 Cl Pb2 90.08(15) . 6_565 ?
Pb1 Cl Pb2 115.35(18) . 6_565 ?
Pb3 Cl Pb2 158.88(19) 2_655 6_565 ?
Pb2 Cl Pb3 85.12(15) 1_554 6_565 ?
Pb3 Cl Pb3 128.58(17) . 6_565 ?
Pb1 Cl Pb3 160.37(18) . 6_565 ?
Pb3 Cl Pb3 104.31(15) 2_655 6_565 ?
Pb2 Cl Pb3 69.94(12) 6_565 6_565 ?
Pb2 Cl OW 152.0(2) 1_554 . ?
Pb3 Cl OW 29.8(3) . . ?
Pb1 Cl OW 100.8(3) . . ?
Pb3 Cl OW 85.56(18) 2_655 . ?
Pb2 Cl OW 75.6(2) 6_565 . ?
Pb3 Cl OW 98.8(3) 6_565 . ?
Pb2 Cl H 143.8(13) 1_554 . ?
Pb3 Cl H 35.2(7) . . ?

Pb1 Cl H 104.7(6) . . ?
Pb3 Cl H 94.7(12) 2_655 . ?
Pb2 Cl H 66.3(12) 6_565 . ?
Pb3 Cl H 94.7(6) 6_565 . ?
OW Cl H 9.3(11) . . ?
C O1 Pb3 126.7(3) . 2_655 ?
C O1 Pb3 126.7(3) . . ?
Pb3 O1 Pb3 106.6(6) 2_655 . ?
C O1 Pb1 89.5(3) . . ?
Pb3 O1 Pb1 95.5(2) 2_655 . ?
Pb3 O1 Pb1 85.10(16) . . ?
C O1 Pb1 89.5(3) . 2_655 ?
Pb3 O1 Pb1 85.10(16) 2_655 2_655 ?
Pb3 O1 Pb1 95.5(2) . 2_655 ?
Pb1 O1 Pb1 179.0(6) . 2_655 ?
C O2 Pb3 128.5(10) 1_565 6_565 ?
C O2 Pb1 108.4(11) 1_565 1_565 ?
Pb3 O2 Pb1 108.3(4) 6_565 1_565 ?
C O2 Pb1 100.0(6) 1_565 6_566 ?
Pb3 O2 Pb1 116.6(4) 6_565 6_566 ?
Pb1 O2 Pb1 87.3(3) 1_565 6_566 ?
C O2 Pb3 64.2(10) 1_565 5_666 ?
Pb3 O2 Pb3 91.2(4) 6_565 5_666 ?
Pb1 O2 Pb3 157.8(4) 1_565 5_666 ?
Pb1 O2 Pb3 74.2(2) 6_566 5_666 ?
Te O3 Pb1 117.9(5) . 4_655 ?
Te O3 Pb2 101.9(4) . 1_554 ?
Pb1 O3 Pb2 138.0(4) 4_655 1_554 ?
Te O3 Pb2 100.5(4) . 6_565 ?
Pb1 O3 Pb2 88.8(3) 4_655 6_565 ?
Pb2 O3 Pb2 96.9(3) 1_554 6_565 ?
Te O3 Pb1 103.4(4) . 7_655 ?
Pb1 O3 Pb1 86.1(3) 4_655 7_655 ?
Pb2 O3 Pb1 71.5(2) 1_554 7_655 ?
Pb2 O3 Pb1 155.1(3) 6_565 7_655 ?
Te O4 Pb3 105.4(4) 7_656 . ?
Te O4 Pb2 107.3(4) 7_656 . ?
Pb3 O4 Pb2 141.7(5) . . ?
Te O4 Pb1 105.9(4) 7_656 1_556 ?
Pb3 O4 Pb1 110.6(3) . 1_556 ?
Pb2 O4 Pb1 78.9(2) . 1_556 ?
Te O4 Pb1 62.4(3) 7_656 6_556 ?
Pb3 O4 Pb1 76.0(2) . 6_556 ?
Pb2 O4 Pb1 138.0(4) . 6_556 ?
Pb1 O4 Pb1 66.97(16) 1_556 6_556 ?
Te O5 Pb1 132.8(4) . . ?
Te O5 Pb2 102.9(4) . 1_554 ?
Pb1 O5 Pb2 110.8(4) . 1_554 ?
Te O5 Pb2 98.4(4) . 7_656 ?
Pb1 O5 Pb2 98.4(3) . 7_656 ?
Pb2 O5 Pb2 112.0(3) 1_554 7_656 ?
Te O6 Pb1 132.4(4) 7_656 . ?
Te O6 Pb3 101.3(4) 7_656 . ?
Pb1 O6 Pb3 114.8(4) . . ?

Te O6 Pb1 92.4(3) 7_656 6_556 ?
Pb1 O6 Pb1 108.8(3) . 6_556 ?
Pb3 O6 Pb1 101.2(3) . 6_556 ?
Te O7 Te 102.7(4) 7_656 . ?
Te O7 Pb2 143.4(4) 7_656 6_565 ?
Te O7 Pb2 111.7(4) . 6_565 ?
Te O7 Pb1 83.8(3) 7_656 7_656 ?
Te O7 Pb1 79.9(3) . 7_656 ?
Pb2 O7 Pb1 90.1(2) 6_565 7_656 ?
Te O7 Pb3 62.4(2) 7_656 . ?
Te O7 Pb3 138.1(4) . . ?
Pb2 O7 Pb3 97.1(2) 6_565 . ?
Pb1 O7 Pb3 131.4(2) 7_656 . ?
Te O7 Pb2 66.1(2) 7_656 . ?
Te O7 Pb2 140.6(4) . . ?
Pb2 O7 Pb2 79.19(19) 6_565 . ?
Pb1 O7 Pb2 61.80(14) 7_656 . ?
Pb3 O7 Pb2 72.51(15) . . ?
Te O7 Pb1 73.2(3) 7_656 . ?
Te O7 Pb1 76.8(3) . . ?
Pb2 O7 Pb1 125.8(3) 6_565 . ?
Pb1 O7 Pb1 142.5(2) 7_656 . ?
Pb3 O7 Pb1 61.53(14) . . ?
Pb2 O7 Pb1 128.8(2) . . ?
Te O7 Pb2 133.9(4) 7_656 1_554 ?
Te O7 Pb2 61.1(2) . 1_554 ?
Pb2 O7 Pb2 76.2(2) 6_565 1_554 ?
Pb1 O7 Pb2 128.6(2) 7_656 1_554 ?
Pb3 O7 Pb2 99.6(2) . 1_554 ?
Pb2 O7 Pb2 153.1(3) . 1_554 ?
Pb1 O7 Pb2 61.42(13) . 1_554 ?
H OW Pb3 121(10) . . ?
H OW Pb3 102(10) . 2_656 ?
Pb3 OW Pb3 107.7(9) . 2_656 ?
H OW Cl 107(10) . . ?
Pb3 OW Cl 37.29(16) . . ?
Pb3 OW Cl 143.3(7) 2_656 . ?
H OW H 0(6) . . ?
Pb3 OW H 121(10) . . ?
Pb3 OW H 102(10) 2_656 . ?
Cl OW H 107(10) . . ?

_diffrn_measured_fraction_theta_max 0.997
_diffrn_reflns_theta_full 23.24
_diffrn_measured_fraction_theta_full 0.997
_refine_diff_density_max 1.395
_refine_diff_density_min -1.327
_refine_diff_density_rms 0.305