Electronic Supplementary Information for Dalton Transactions

Electronic Supplementary Information (ESI)

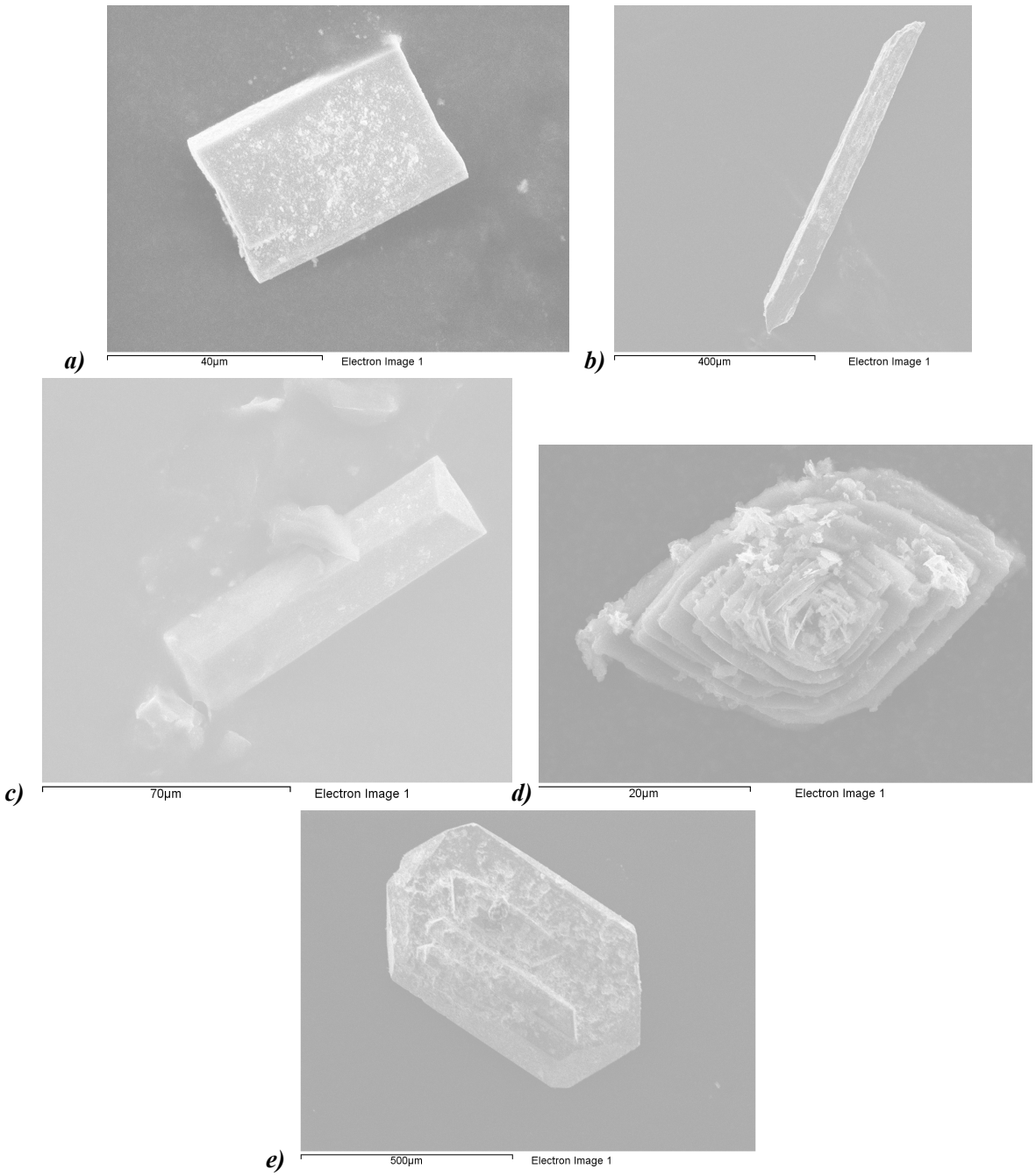

Figure 1: *EDS images for* ***a)*** *$[CsCe_2F_8[F.H_2O]]$,* ***b)*** *$[NH_4]_5[H_2O]_2[Ce^{IV}{}_4(AsO_4)_6(H_2O)F_3]$,* ***c)*** *$Ce[AsO_4]F$,* ***d)*** *$Ce[AsO_4][H_2O]F$ and* ***e)*** *$[NH_4][Ce^{IV}F_2(AsO_4)]$*

[$CsCe_2F_8[F.H_2O]$]

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 'Cs'  'Cs'  -0.3680   2.1192
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ce'  'Ce'  -0.2486   2.6331
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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_symmetry_space_group_name_H-M    C2/c

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 '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'

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_exptl_crystal_size_min           0.02
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_exptl_crystal_density_method     'not measured'
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_computing_cell_refinement
'DENZO (Otwinowski & Minor, 1997) & COLLECT (Hooft, R.W.W., 1998)'
_computing_data_reduction
'DENZO (Otwinowski & Minor, 1997) & COLLECT (Hooft, R.W.W., 1998)'
_computing_structure_solution   'SHELXS-97 (Sheldrick, 1997)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics     'CAMERON (Watkin, et al., 1993)'
_computing_publication_material   'WINGX (Farrugia, 1998)'

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;
 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(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.

 An isotropic thermal restraint was used to reduce the prolate nature of
 the oxygen temperature factor.

 The O1/F5 site is split based on charge balance backed up by IR and EDX
 analysis. The hydrogen atom shave been included in the formula, but not
 the refinement.
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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0681P)^2^+9.3573P] where P=(Fo^2^+2Fc^2^)/3'
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 _atom_site_occupancy
 _atom_site_symmetry_multiplicity
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Ce1 Ce 0.21372(3) 1.09670(6) 0.29446(6) 0.0063(3) Uani 1 1 d . . .
F3 F 0.3343(3) 1.1807(6) 0.5688(5) 0.0096(9) Uani 1 1 d . . .
F4 F 0.1851(3) 1.0489(7) 0.0131(5) 0.0105(9) Uani 1 1 d . . .
O1 O 0.0465(5) 1.0894(8) 0.1517(8) 0.0169(14) Uani 0.50 1 d P . .
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 _atom_site_aniso_U_23
 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
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F2 0.008(2) 0.011(2) 0.009(2) 0.0011(17) 0.0049(17) 0.0016(19)
Cs1 0.0069(5) 0.0179(6) 0.0102(5) 0.000 0.0027(4) 0.000
Ce1 0.0056(4) 0.0090(4) 0.0042(4) -0.00036(13) 0.0022(3) -0.00010(14)
F3 0.005(2) 0.016(3) 0.007(2) 0.0002(19) 0.0025(16) 0.0030(19)
F4 0.014(2) 0.010(2) 0.007(2) -0.0015(18) 0.0042(18) -0.003(2)
O1 0.014(3) 0.026(4) 0.009(3) -0.004(2) 0.005(2) -0.007(2)
F5 0.014(3) 0.026(4) 0.009(3) -0.004(2) 0.005(2) -0.007(2)

_geom_special_details
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 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
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 _geom_bond_site_symmetry_2
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F1 Cs1 3.386(4) . ?
F2 Ce1 2.283(4) . ?
F2 Ce1 2.304(4) 4 ?
F2 Cs1 2.993(4) . ?
Cs1 F2 2.993(4) 2_655 ?
Cs1 F3 3.036(4) 6_575 ?
Cs1 F3 3.036(4) 5_676 ?
Cs1 F1 3.070(4) 5_676 ?
Cs1 F1 3.070(4) 6_575 ?
Cs1 F1 3.386(4) 2_655 ?
Ce1 F4 2.262(4) . ?
Ce1 F3 2.270(4) 7_576 ?
Ce1 O1 2.285(6) . ?
Ce1 F3 2.288(4) . ?
Ce1 F2 2.304(4) 4_545 ?
Ce1 F4 2.348(4) 6_576 ?
Ce1 F1 2.411(4) 4 ?
F3 Ce1 2.270(4) 7_576 ?
F3 Cs1 3.036(4) 5_676 ?
F4 Ce1 2.348(4) 6_575 ?


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 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_1
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Ce1 F1 Cs1 119.70(15) 4_545 5_676 ?
Ce1 F1 Cs1 108.42(14) . . ?
Ce1 F1 Cs1 108.54(15) 4_545 . ?
Cs1 F1 Cs1 88.87(11) 5_676 . ?
Ce1 F2 Ce1 114.14(18) . 4 ?
Ce1 F2 Cs1 121.47(17) . . ?
Ce1 F2 Cs1 122.48(17) 4 . ?
F2 Cs1 F2 131.49(17) 2_655 . ?
F2 Cs1 F3 142.13(11) 2_655 6_575 ?
F2 Cs1 F3 75.52(11) . 6_575 ?
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F2 Cs1 F3 142.13(11) . 5_676 ?
F3 Cs1 F3 97.93(17) 6_575 5_676 ?
F2 Cs1 F1 77.81(11) 2_655 5_676 ?
F2 Cs1 F1 102.22(11) . 5_676 ?
F3 Cs1 F1 127.76(11) 6_575 5_676 ?
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F2 Cs1 F1 102.22(11) 2_655 6_575 ?
F2 Cs1 F1 77.81(11) . 6_575 ?
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F3 Cs1 F1 127.76(11) 5_676 6_575 ?
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F2 Cs1 F1 51.20(11) . . ?
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F3 Cs1 F4 83.61(11) 5_676 8_576 ?
F1 Cs1 F4 47.52(10) 5_676 8_576 ?
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F1 Cs1 F4 132.53(10) 5_676 7_575 ?
F1 Cs1 F4 47.52(10) 6_575 7_575 ?
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F2 Cs1 O1 84.81(13) . 3 ?
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F3 Cs1 O1 121.20(13) 5_676 3 ?
F1 Cs1 O1 95.92(12) 5_676 3 ?
F1 Cs1 O1 84.13(12) 6_575 3 ?
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O1 Ce1 Ce1 106.04(15) . 7_576 ?
F3 Ce1 Ce1 33.07(10) . 7_576 ?
F2 Ce1 Ce1 134.58(10) 4_545 7_576 ?
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F4 Ce1 Ce1 81.53(12) . 4 ?
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O1 Ce1 Ce1 106.01(14) . 4 ?
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F2 Ce1 Ce1 153.43(10) 4_545 4 ?
F4 Ce1 Ce1 137.02(12) 6_576 4 ?
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$[NH_4]_{10}[H_2O]_4[Ce^{IV}_8(AsO_4)_{12}(H_2O)_2F_6]$

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_chemical_melting_point           ?
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 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ce'  'Ce'  -0.2486   2.6331
 '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'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'F'  'F'   0.0171   0.0103
 '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'

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_symmetry_space_group_name_H-M    P-1
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 '-x, -y, -z'

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_cell_angle_gamma                 114.293(2)
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_diffrn_reflns_limit_h_min        -11
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_diffrn_reflns_limit_k_min        -11
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_diffrn_reflns_limit_l_max        22
_diffrn_reflns_theta_min          3.00
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_reflns_number_total              5106
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'COLLECT (Hooft, R.W.W., 1998)'
_computing_cell_refinement
'DENZO (Otwinowski & Minor, 1997) & COLLECT (Hooft, R.W.W., 1998)'
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'DENZO (Otwinowski & Minor, 1997) & COLLECT (Hooft, R.W.W., 1998)'
_computing_structure_solution   'SHELXS-97 (Sheldrick, 1997)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 2008)'
_computing_molecular_graphics     'CAMERON (Watkin, et al., 1993)'
_computing_publication_material   'WINGX (Farrugia, 1998)'

_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\s(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.

 An isotropic thermal restraint was used to reduce the oblate nature of
 the oxygen temperature factors for O22 and O52.
 The hydrogen atoms shave been included in the formula, but not the
 refinement.

;

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_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0307P)^2^+9.7864P] where P=(Fo^2^+2Fc^2^)/3'
_atom_sites_solution_primary      direct
_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    none
_refine_ls_hydrogen_treatment     none
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
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_refine_ls_number_parameters      406
_refine_ls_number_restraints      12
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_refine_ls_wR_factor_ref          0.0851
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_refine_ls_wR_factor_gt           0.0829
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As3 As -0.10710(8) 0.51862(7) 0.13040(3) 0.00599(15) Uani 1 1 d . . .
As4 As 0.12901(8) 1.00616(7) 0.37343(3) 0.00594(15) Uani 1 1 d . . .
As5 As -0.00969(8) 0.54618(7) 0.36777(3) 0.00576(15) Uani 1 1 d . . .
As6 As 0.34032(8) 0.64637(7) 0.11259(3) 0.00515(15) Uani 1 1 d . . .
Ce1 Ce 0.26309(4) 0.82953(4) 0.275444(19) 0.00556(11) Uani 1 1 d . . .
Ce2 Ce -0.03654(4) 0.28594(4) 0.033012(19) 0.00527(11) Uani 1 1 d . . .
Ce3 Ce 0.04370(4) 1.22606(4) 0.473955(19) 0.00561(11) Uani 1 1 d . . .
Ce4 Ce -0.24543(4) 0.69527(4) 0.222506(19) 0.00533(11) Uani 1 1 d . . .
N1 N -0.1954(7) 1.1504(7) 0.2486(3) 0.0141(12) Uani 1 1 d . . .
N2 N 0.6079(7) 0.2154(7) 0.4943(3) 0.0178(13) Uani 1 1 d . . .
N3 N 0.2292(8) 0.3768(9) 0.2545(4) 0.0304(17) Uani 1 1 d . . .
N4 N 0.4600(8) 0.4621(9) 0.4071(3) 0.037(2) Uani 1 1 d . . .
N5 N 0.5624(9) 0.2970(8) 0.3310(4) 0.0344(18) Uani 1 1 d . . .
O11 O 0.4743(5) 0.8174(5) 0.3660(2) 0.0087(9) Uani 1 1 d . . .
O12 O 0.7765(5) 1.0682(5) 0.4129(2) 0.0090(9) Uani 1 1 d . . .
O13 O 0.7183(6) 0.8455(6) 0.2998(2) 0.0129(10) Uani 1 1 d . . .
O14 O 0.7255(6) 0.7645(5) 0.4434(2) 0.0113(10) Uani 1 1 d . . .
O21 O -0.1352(5) 0.8991(5) 0.1546(2) 0.0100(10) Uani 1 1 d . . .
O22 O 0.0696(5) 1.1544(5) 0.1107(2) 0.0078(9) Uani 1 1 d U . .
O23 O 0.2064(5) 0.9925(5) 0.1968(2) 0.0093(9) Uani 1 1 d . . .
O24 O 0.0167(6) 0.8628(5) 0.0508(3) 0.0135(10) Uani 1 1 d . . .
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O32 O -0.2954(5) 0.5059(5) 0.1196(2) 0.0106(10) Uani 1 1 d . . .
O33 O -0.0883(6) 0.3537(5) 0.1483(2) 0.0099(10) Uani 1 1 d . . .
O34 O -0.0410(6) 0.5409(5) 0.0524(2) 0.0098(10) Uani 1 1 d . . .
O41 O 0.0257(5) 0.8625(5) 0.3008(2) 0.0098(10) Uani 1 1 d . . .
O42 O 0.3162(5) 1.0125(5) 0.3848(3) 0.0111(10) Uani 1 1 d . . .
O43 O 0.1230(6) 1.1793(5) 0.3622(2) 0.0102(10) Uani 1 1 d . . .
O44 O 0.0503(6) 0.9703(5) 0.4474(2) 0.0091(9) Uani 1 1 d . . .
O51 O -0.1743(6) 0.5444(6) 0.3042(3) 0.0127(10) Uani 1 1 d . . .
O52 O 0.0316(6) 0.6623(5) 0.4477(2) 0.0113(10) Uani 1 1 d U . .
O53 O -0.0596(6) 0.3599(5) 0.3834(2) 0.0098(9) Uani 1 1 d . . .
O54 O 0.1559(5) 0.6172(5) 0.3348(2) 0.0106(10) Uani 1 1 d . . .
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O62 O 0.2810(5) 0.7447(5) 0.0448(2) 0.0086(9) Uani 1 1 d . . .
O63 O 0.5407(5) 0.7026(5) 0.1253(2) 0.0069(9) Uani 1 1 d . . .
O64 O 0.2330(5) 0.4514(5) 0.0861(2) 0.0079(9) Uani 1 1 d . . .
O1 O -0.2730(5) 0.0519(5) 0.0576(2) 0.0112(10) Uani 1 1 d . . .
OW1 O 0.4637(6) 0.0581(5) 0.1049(3) 0.0146(10) Uani 1 1 d . . .
OW2 O 0.4077(7) 0.2982(7) 0.0292(3) 0.0299(13) Uani 1 1 d . . .
F1 F -0.4696(5) 0.5136(6) 0.2367(2) 0.0245(10) Uani 1 1 d . . .
F2 F 0.4925(5) 1.0165(5) 0.2596(2) 0.0174(9) Uani 1 1 d . . .
F3 F 0.2421(5) 1.4588(5) 0.4827(2) 0.0216(9) Uani 1 1 d . . .

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As2 0.0081(3) 0.0060(3) 0.0054(3) 0.0017(2) 0.0030(3) 0.0043(3)
As3 0.0077(3) 0.0056(3) 0.0057(3) 0.0004(2) 0.0028(2) 0.0033(3)
As4 0.0071(3) 0.0062(3) 0.0050(3) 0.0002(2) 0.0026(3) 0.0028(3)
As5 0.0074(3) 0.0058(3) 0.0048(3) 0.0009(2) 0.0021(2) 0.0032(3)
As6 0.0052(3) 0.0062(3) 0.0047(3) 0.0004(2) 0.0016(2) 0.0030(3)
Ce1 0.0060(2) 0.00652(19) 0.00474(18) 0.00052(14) 0.00194(14) 0.00304(15)
Ce2 0.0068(2) 0.00501(19) 0.00491(19) 0.00059(14) 0.00226(14) 0.00311(15)
Ce3 0.0071(2) 0.00560(19) 0.00481(19) 0.00053(14) 0.00197(14) 0.00318(15)
Ce4 0.0061(2) 0.00570(19) 0.00489(18) 0.00036(14) 0.00187(14) 0.00298(15)
N1 0.017(3) 0.012(3) 0.010(3) 0.003(2) 0.002(2) 0.005(3)
N2 0.010(3) 0.018(3) 0.018(3) 0.004(3) -0.003(2) 0.002(3)
N3 0.015(4) 0.039(4) 0.034(4) 0.025(3) 0.005(3) 0.009(3)
N4 0.022(4) 0.049(5) 0.010(3) -0.001(3) 0.007(3) -0.014(3)
N5 0.034(4) 0.016(4) 0.028(4) 0.014(3) -0.004(3) -0.007(3)
O11 0.005(2) 0.013(2) 0.008(2) 0.0035(18) 0.0016(18) 0.0046(19)
O12 0.011(2) 0.010(2) 0.006(2) 0.0021(18) 0.0011(18) 0.005(2)
O13 0.014(3) 0.019(3) 0.010(2) -0.0020(19) 0.0052(19) 0.010(2)
O14 0.009(2) 0.012(2) 0.012(2) 0.0036(19) -0.0004(19) 0.005(2)
O21 0.007(2) 0.012(2) 0.015(2) 0.0017(19) 0.0056(19) 0.005(2)
O22 0.011(2) 0.004(2) 0.008(2) 0.0040(16) 0.0023(17) 0.0031(17)
O23 0.007(2) 0.009(2) 0.013(2) 0.0066(18) 0.0022(18) 0.0043(19)
O24 0.021(3) 0.011(2) 0.012(2) -0.0006(19) 0.006(2) 0.009(2)
O31 0.006(2) 0.009(2) 0.008(2) -0.0022(18) 0.0003(18) 0.0040(19)
O32 0.008(2) 0.011(2) 0.012(2) -0.0031(19) 0.0026(19) 0.0034(19)
O33 0.013(2) 0.010(2) 0.011(2) 0.0012(18) 0.0061(19) 0.007(2)
O34 0.016(3) 0.011(2) 0.006(2) 0.0013(18) 0.0062(19) 0.007(2)
O41 0.011(2) 0.009(2) 0.007(2) -0.0047(18) 0.0006(18) 0.004(2)
O42 0.007(2) 0.011(2) 0.014(2) -0.0024(19) 0.0020(19) 0.004(2)
O43 0.011(2) 0.010(2) 0.012(2) 0.0054(18) 0.0076(19) 0.005(2)
O44 0.014(2) 0.010(2) 0.006(2) 0.0003(18) 0.0059(19) 0.006(2)
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O64 0.011(2) 0.006(2) 0.007(2) 0.0003(17) 0.0014(18) 0.0047(19)
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OW1 0.017(3) 0.012(2) 0.017(2) 0.0026(19) 0.007(2) 0.006(2)
OW2 0.022(3) 0.028(3) 0.035(3) 0.001(3) 0.004(3) 0.008(3)
F1 0.016(2) 0.038(3) 0.025(2) 0.021(2) 0.0092(19) 0.015(2)
F2 0.008(2) 0.020(2) 0.017(2) 0.0099(17) 0.0007(16) 0.0013(17)
F3 0.016(2) 0.011(2) 0.031(2) 0.0099(18) 0.0028(19) 0.0016(18)

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
;

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As2 O21 1.692(4) . ?
As2 O24 1.696(4) . ?
As3 O31 1.675(4) . ?
As3 O33 1.683(4) . ?
As3 O32 1.683(4) . ?
As3 O34 1.689(4) . ?
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As3 Ce2 3.1960(7) . ?
As4 O41 1.678(4) . ?
As4 O44 1.684(4) . ?
As4 O43 1.689(4) . ?
As4 O42 1.694(4) . ?
As4 Ce1 3.2279(7) . ?
As4 Ce3 3.2287(7) . ?
As5 O53 1.690(4) . ?
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As5 O52 1.691(4) . ?
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As6 O61 1.687(4) . ?
As6 O64 1.700(4) . ?
As6 O62 1.704(4) . ?
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Ce1 O61 2.197(4) . ?
Ce1 F2 2.252(4) . ?
Ce1 O23 2.283(4) . ?
Ce1 O54 2.295(5) . ?
Ce1 O11 2.311(4) . ?
Ce1 O31 2.382(4) . ?
Ce1 O42 2.454(4) . ?
Ce1 O41 2.522(4) . ?
Ce2 O24 2.170(4) 2_565 ?
Ce2 O22 2.245(4) 1_545 ?
Ce2 O62 2.292(4) 2_565 ?
Ce2 O64 2.302(4) . ?
Ce2 O34 2.329(4) 2_565 ?
Ce2 O33 2.430(4) . ?
Ce2 O34 2.467(4) . ?
Ce2 O1 2.562(5) . ?
Ce2 Ce2 4.1135(7) 2_565 ?
Ce3 O52 2.186(4) 2_576 ?
Ce3 F3 2.203(4) . ?
Ce3 O14 2.295(5) 2_676 ?
Ce3 O12 2.298(5) 1_455 ?
Ce3 O53 2.386(4) 1_565 ?
Ce3 O44 2.404(4) 2_576 ?
Ce3 O43 2.450(4) . ?
Ce3 O44 2.504(4) . ?
Ce4 O13 2.181(4) 1_455 ?
Ce4 F1 2.188(4) . ?
Ce4 O51 2.278(5) . ?
Ce4 O21 2.346(5) . ?
Ce4 O63 2.376(4) 1_455 ?
Ce4 O32 2.413(4) . ?
Ce4 O41 2.428(4) . ?
Ce4 O31 2.519(4) . ?
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O22 Ce2 2.245(4) 1_565 ?
O24 Ce2 2.170(4) 2_565 ?
O34 Ce2 2.329(4) 2_565 ?
O44 Ce3 2.404(4) 2_576 ?
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O11 As1 O14 105.5(2) . . ?
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O13 As1 O14 110.1(2) . . ?
O23 As2 O22 106.9(2) . . ?
O23 As2 O21 115.3(2) . . ?
O22 As2 O21 105.7(2) . . ?
O23 As2 O24 110.9(2) . . ?
O22 As2 O24 109.6(2) . . ?
O21 As2 O24 108.3(2) . . ?
O31 As3 O33 119.0(2) . . ?
O31 As3 O32 98.9(2) . . ?
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O31 As3 O34 112.5(2) . . ?
O33 As3 O34 97.2(2) . . ?
O32 As3 O34 115.9(2) . . ?
O31 As3 Ce4 51.64(15) . . ?
O33 As3 Ce4 126.52(15) . . ?
O32 As3 Ce4 48.01(15) . . ?
O34 As3 Ce4 136.23(15) . . ?
O31 As3 Ce2 138.71(15) . . ?
O33 As3 Ce2 48.40(14) . . ?
O32 As3 Ce2 122.33(15) . . ?
O34 As3 Ce2 49.71(15) . . ?
Ce4 As3 Ce2 168.81(3) . . ?
O41 As4 O44 112.8(2) . . ?
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O44 As4 O42 117.4(2) . . ?
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O44 As4 Ce1 135.48(15) . . ?
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O44 As4 Ce3 50.00(15) . . ?
O43 As4 Ce3 48.16(15) . . ?
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Ce1 As4 Ce3 171.76(2) . . ?
O53 As5 O54 111.5(2) . . ?
O53 As5 O52 111.1(2) . . ?
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O53 As5 O51 106.0(2) . . ?
O54 As5 O51 111.0(2) . . ?
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O63 As6 O61 111.2(2) . . ?
O63 As6 O64 111.6(2) . . ?
O61 As6 O64 107.5(2) . . ?
O63 As6 O62 106.8(2) . . ?
O61 As6 O62 109.3(2) . . ?
O64 As6 O62 110.5(2) . . ?
O61 Ce1 F2 82.35(16) . . ?
O61 Ce1 O23 96.91(16) . . ?
F2 Ce1 O23 68.95(15) . . ?
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F2 Ce1 O54 145.57(15) . . ?
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F2 Ce1 O11 74.11(15) . . ?
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O61 Ce1 O31 76.06(16) . . ?
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O61 Ce1 O42 161.11(16) . . ?
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F2 Ce1 As4 105.22(11) . . ?
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O22 Ce2 O34 137.85(16) 1_545 2_565 ?
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 'x-1/2, y, -z-1/2'
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SADABS V2.10 (Sheldrick, G.M., 2003)
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SADABS was used to perform the Absorption correction
Parameter refinement on 5713 reflections reduced R(int) from 0.2086 to 0.0973
Ratio of minimum to maximum apparent transmission:  0.710537
The given Tmin and Tmax were generated using the SHELX SIZE command
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_diffrn_reflns_number             5482
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_diffrn_reflns_av_sigmaI/netI     0.0370
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_diffrn_reflns_limit_h_max        11
_diffrn_reflns_limit_k_min        -9
_diffrn_reflns_limit_k_max        8
_diffrn_reflns_limit_l_min        -8
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
 goodness of fit S are based on F^2^, conventional R-factors R are based
 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2\s(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;

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_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
 'calc w=1/[\s^2^(Fo^2^)+(0.0153P)^2^+16.4767P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    none
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O3 O 0.2873(10) 0.7500 -0.1025(13) 0.0097(9) Uani 1 2 d S . .
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 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
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O2 Ce1 O1 138.0(2) 6_656 4_564 ?
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 'As'  'As'   0.0499   2.0058
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ce'  'Ce'  -0.2486   2.6331
 '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'

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_symmetry_space_group_name_H-M    P21/n

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

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_cell_length_b                    7.5118(5)
_cell_length_c                    11.8183(8)
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_cell_angle_beta                  97.740(4)
_cell_angle_gamma                 90.00
_cell_volume                      447.72(5)
_cell_formula_units_Z             4
_cell_measurement_temperature     120(2)
_cell_measurement_reflns_used     10067
_cell_measurement_theta_min       2.91
_cell_measurement_theta_max       27.48

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_exptl_crystal_size_min           0.02
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_exptl_crystal_density_diffrn     4.689
_exptl_crystal_density_method     'not measured'
_exptl_crystal_F_000              568
_exptl_absorpt_coefficient_mu     17.453
_exptl_absorpt_correction_type    multi-scan
_exptl_absorpt_correction_T_min   0.4757
_exptl_absorpt_correction_T_max   0.7216
_exptl_absorpt_process_details    'SADABS V2.10 (Sheldrick, G.M., 2003)'

_exptl_special_details
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_diffrn_radiation_wavelength      0.71073
_diffrn_radiation_type            MoK\a
_diffrn_radiation_source          'Bruker Nonius FR591 Rotating Anode'
_diffrn_radiation_monochromator  '10cm confocal mirrors'
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_diffrn_measurement_method        '\f & \w scans to fill the asymmetric unit'
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_diffrn_standards_number   0
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_diffrn_standards_interval_time   ?
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_diffrn_reflns_number             4520
_diffrn_reflns_av_R_equivalents   0.1076
_diffrn_reflns_av_sigmaI/netI     0.0682
_diffrn_reflns_limit_h_min        -6
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_diffrn_reflns_limit_k_min        -8
_diffrn_reflns_limit_k_max        8
_diffrn_reflns_limit_l_min        -14
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_diffrn_reflns_theta_min          3.22
_diffrn_reflns_theta_max          25.02
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_reflns_threshold_expression      >2\s(I)

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_computing_cell_refinement
'DENZO (Otwinowski & Minor, 1997) & COLLECT (Hooft, R.W.W., 1998)'
_computing_data_reduction
'DENZO (Otwinowski & Minor, 1997) & COLLECT (Hooft, R.W.W., 1998)'
_computing_structure_solution   'SHELXS-97 (Sheldrick, 1997)'
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_computing_molecular_graphics     'CAMERON (Watkin, et al., 1993)'
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_computing_publication_material   'WINGX (Farrugia, 1998)'

_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\s(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.

 The hydrogen atoms have been included in the formula, but not the
 refinement.
;

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
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_refine_ls_extinction_method      none
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_refine_ls_number_parameters      43
_refine_ls_number_restraints      0
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 _atom_site_occupancy
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 _atom_site_calc_flag
 _atom_site_refinement_flags
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As1 As 0.7900(5) 0.8621(3) 0.3868(2) 0.0086(6) Uani 1 1 d . . .
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F1 F 0.133(2) 0.5038(17) 0.3230(11) 0.0092(14) Uani 1 1 d . . .
O1 O -0.123(3) 0.888(2) 0.0779(13) 0.0092(14) Uani 1 1 d . . .
O2 O 0.612(3) 0.710(2) 0.3067(13) 0.0092(14) Uani 1 1 d . . .
O3 O 0.617(3) 1.049(2) 0.3940(13) 0.0092(14) Uani 1 1 d . . .
O4 O 0.877(3) 0.782(2) 0.5211(13) 0.0092(14) Uani 1 1 d . . .
O5 O 1.069(3) 0.901(2) 0.3272(13) 0.0092(14) Uani 1 1 d . . .

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 _atom_site_aniso_U_12
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As1 0.0097(12) 0.0067(12) 0.0093(12) -0.0006(9) 0.0010(9) 0.0012(9)
F1 0.011(3) 0.007(3) 0.010(3) 0.003(3) 0.000(3) 0.003(3)
O1 0.011(3) 0.007(3) 0.010(3) 0.003(3) 0.000(3) 0.003(3)
O2 0.011(3) 0.007(3) 0.010(3) 0.003(3) 0.000(3) 0.003(3)
O3 0.011(3) 0.007(3) 0.010(3) 0.003(3) 0.000(3) 0.003(3)
O4 0.011(3) 0.007(3) 0.010(3) 0.003(3) 0.000(3) 0.003(3)
O5 0.011(3) 0.007(3) 0.010(3) 0.003(3) 0.000(3) 0.003(3)

_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
;

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Ce1 O4 2.246(15) 4_575 ?
Ce1 F1 2.275(13) . ?
Ce1 O2 2.290(15) . ?
Ce1 F1 2.376(13) 2 ?
Ce1 O5 2.389(16) 1_455 ?
Ce1 O1 2.445(15) . ?
Ce1 O5 2.555(16) 2_645 ?
As1 O3 1.664(16) . ?
As1 O2 1.671(16) . ?
As1 O5 1.695(16) . ?
As1 O4 1.700(15) . ?
F1 Ce1 2.376(13) 2_545 ?
O3 Ce1 2.186(15) 2 ?
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O4 Ce1 2.246(15) 4_676 ?
O5 Ce1 2.389(16) 1_655 ?
O5 Ce1 2.555(16) 2_655 ?

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 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
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O3 Ce1 F1 75.3(5) 2_545 . ?
O4 Ce1 F1 140.2(5) 4_575 . ?
O3 Ce1 O2 147.8(6) 2_545 . ?
O4 Ce1 O2 98.2(5) 4_575 . ?
F1 Ce1 O2 79.4(5) . . ?
O3 Ce1 F1 135.9(5) 2_545 2 ?
O4 Ce1 F1 75.5(5) 4_575 2 ?
F1 Ce1 F1 139.6(3) . 2 ?
O2 Ce1 F1 76.1(5) . 2 ?
O3 Ce1 O5 110.0(6) 2_545 1_455 ?
O4 Ce1 O5 139.7(6) 4_575 1_455 ?
F1 Ce1 O5 80.0(5) . 1_455 ?
O2 Ce1 O5 84.7(5) . 1_455 ?
F1 Ce1 O5 66.1(5) 2 1_455 ?
O3 Ce1 O1 67.2(6) 2_545 . ?
O4 Ce1 O1 79.5(5) 4_575 . ?
F1 Ce1 O1 124.2(5) . . ?
O2 Ce1 O1 145.0(6) . . ?
F1 Ce1 O1 69.5(5) 2 . ?
O5 Ce1 O1 76.1(5) 1_455 . ?
O3 Ce1 O5 78.2(6) 2_545 2_645 ?
O4 Ce1 O5 76.3(5) 4_575 2_645 ?
F1 Ce1 O5 64.9(5) . 2_645 ?
O2 Ce1 O5 73.0(5) . 2_645 ?
F1 Ce1 O5 134.2(5) 2 2_645 ?
O5 Ce1 O5 141.0(3) 1_455 2_645 ?
O1 Ce1 O5 137.8(5) . 2_645 ?
O3 Ce1 Ce1 133.5(4) 2_545 2 ?
O4 Ce1 Ce1 104.7(4) 4_575 2 ?
F1 Ce1 Ce1 112.8(3) . 2 ?
O2 Ce1 Ce1 75.2(4) . 2 ?
F1 Ce1 Ce1 29.4(3) 2 2 ?
O5 Ce1 Ce1 36.9(4) 1_455 2 ?
O1 Ce1 Ce1 71.9(4) . 2 ?
O5 Ce1 Ce1 147.9(3) 2_645 2 ?
O3 Ce1 Ce1 71.4(4) 2_545 2_545 ?
O4 Ce1 Ce1 109.5(4) 4_575 2_545 ?
F1 Ce1 Ce1 30.9(3) . 2_545 ?
O2 Ce1 Ce1 76.7(4) . 2_545 ?
F1 Ce1 Ce1 152.7(3) 2 2_545 ?
O5 Ce1 Ce1 110.3(4) 1_455 2_545 ?
O1 Ce1 Ce1 137.3(4) . 2_545 ?
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O5 Ce1 Ce1 34.2(4) 2_645 2_545 ?
Ce1 Ce1 Ce1 138.07(7) 2 2_545 ?
O3 As1 O2 110.8(8) . . ?
O3 As1 O5 111.0(8) . . ?
O2 As1 O5 107.5(7) . . ?
O3 As1 O4 109.0(8) . . ?
O2 As1 O4 109.7(8) . . ?
O5 As1 O4 108.8(7) . . ?
Ce1 F1 Ce1 119.7(5) . 2_545 ?
As1 O2 Ce1 135.9(9) . . ?
As1 O3 Ce1 144.7(9) . 2 ?
As1 O4 Ce1 136.8(8) . 4_676 ?
As1 O5 Ce1 122.5(8) . 1_655 ?
As1 O5 Ce1 125.1(8) . 2_655 ?
Ce1 O5 Ce1 108.8(6) 1_655 2_655 ?

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_diffrn_reflns_theta_full              25.02
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$[NH_4][Ce^{IV}F_2(AsO_4)]$

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 'As'  'As'   0.0499   2.0058
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Ce'  'Ce'  -0.2486   2.6331
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'F'  'F'   0.0171   0.0103
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 'N'  'N'   0.0061   0.0033
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 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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

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_cell_length_b                    6.0181(2)
_cell_length_c                    7.1315(2)
_cell_angle_alpha                 90.00
_cell_angle_beta                  113.832(2)
_cell_angle_gamma                 90.00
_cell_volume                      266.009(14)
_cell_formula_units_Z             2
_cell_measurement_temperature     120(2)
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_exptl_crystal_F_000              304
_exptl_absorpt_coefficient_mu     14.718
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_diffrn_radiation_source          'Bruker Nonius FR591 Rotating Anode'
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_diffrn_measurement_device_type   'Bruker-Nonius CCD camera on \k-goniostat'
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_diffrn_standards_interval_count  ?
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_diffrn_reflns_number             5124
_diffrn_reflns_av_R_equivalents   0.0441
_diffrn_reflns_av_sigmaI/netI     0.0408
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_diffrn_reflns_limit_k_min        -9
_diffrn_reflns_limit_k_max        9
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_computing_cell_refinement
'DENZO (Otwinowski & Minor, 1997) & COLLECT (Hooft, R.W.W., 1998)'
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'DENZO (Otwinowski & Minor, 1997) & COLLECT (Hooft, R.W.W., 1998)'
_computing_structure_solution   'SHELXS-97 (Sheldrick, 1997)'
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_computing_publication_material   'WINGX (Farrugia, 1998)'

_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\s(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.

 The hydrogen atoms have been included in the formula, but not the
 refinement.
;

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme       calc
_refine_ls_weighting_details
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_refine_ls_wR_factor_gt           0.0973
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_refine_ls_shift/su_mean          0.001

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 _atom_site_refinement_flags
 _atom_site_disorder_assembly
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F1 F 0.6607(4) -0.0040(4) 0.4575(3) 0.0069(4) Uani 1 1 d . . .
O1 O -0.0010(7) 0.2500 0.2596(6) 0.0061(7) Uani 1 2 d SU . .
O2 O -0.2279(5) 0.0258(4) -0.1018(4) 0.0082(5) Uani 1 1 d . . .
O3 O -0.4492(7) 0.2500 0.0904(6) 0.0075(7) Uani 1 2 d S . .
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F1 0.0056(10) 0.0097(10) 0.0063(10) 0.0042(8) 0.0034(8) 0.0034(8)
O1 0.0060(10) 0.0069(10) 0.0047(10) 0.000 0.0014(8) 0.000
O2 0.0057(12) 0.0087(12) 0.0099(12) -0.0051(10) 0.0028(10) -0.0004(10)
O3 0.0055(17) 0.0098(17) 0.0094(17) 0.000 0.0054(15) 0.000
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_geom_special_details
;
 All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes)
```

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 are estimated using the full covariance matrix.  The cell s.u.'s are taken
 into account individually in the estimation of s.u.'s in distances, angles
 and torsion angles; correlations between s.u.'s in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell s.u.'s is used for estimating s.u.'s involving l.s.
planes.
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Ce1 O2 2.167(3) 2 ?
Ce1 O3 2.240(4) 1_655 ?
Ce1 F1 2.331(2) 4_565 ?
Ce1 F1 2.331(2) . ?
Ce1 F1 2.363(2) 2_656 ?
Ce1 F1 2.363(2) 3_656 ?
Ce1 O1 2.486(4) . ?
Ce1 Ce1 3.9827(4) 3_666 ?
Ce1 Ce1 3.9827(4) 3_656 ?
As1 O3 1.671(4) . ?
As1 O1 1.689(4) . ?
As1 O2 1.692(3) . ?
As1 O2 1.692(3) 4_565 ?
F1 Ce1 2.363(2) 3_656 ?
O2 Ce1 2.167(3) 3 ?
O3 Ce1 2.240(4) 1_455 ?

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F1 Ce1 F1 81.95(12) 4_565 . ?
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F1 Ce1 F1 63.92(8) 4_565 2_656 ?
F1 Ce1 F1 112.46(4) . 2_656 ?
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F1 Ce1 Ce1 98.32(6) 4_565 3_656 ?
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