

fluoro-tremolite 1082\_751\_361.cif

```

data_1082_IHQ

_publ_contact_author
;
Roberta Oberti
;
_publ_contact_author_email
;
oberti@crystal.unipv.it
;

loop_
_publ_author_name
_publ_author_address
'Oberti R.'
'CNR-IGG, S.S. Pavia, Pavia, Italy'
'Camara F.'
'Dip.to di Scienze della Terra, Università di Milano, Milan, Italy'
'Bellatreccia F.'
'Dip.to di Scienze, Università Roma Tre, Rome, Italy'
'Radica F.'
'Dip.to di Scienze, Università Roma Tre, Rome, Italy'
'Gianfagna A.'
'Dip.to di Scienze della Terra, Università di Roma La Sapienza, Rome, Italy'
'Boiocchi M.'
'Centro Grandi Strumenti, Università di Pavia, Pavia, Italy'

_publ_section_title
;
Fluoro-tremolite from the Limecrest-Southdown quarry, Sparta, NJ, USA:
crystal structure and crystal chemistry of a newly approved end-members
of the amphibole supergroup and its solid solution with tremolite
;

_audit_creation_method      'manually entered'
_chemical_name_systematic   ?
_chemical_name_mineral
;
fluoro-tremolite
;
_chemical_compound_source
;
Limecrest-Southdown quarry, Sparta, New Jersey, USA
;
_chemical_name_common        ?
_chemical_melting_point     ?
_chemical_formula_moietry    ?
_chemical_formula_sum
'A10.40 Ca1.95 F1.36 Fe0.26 H0.98 Mg4.83 Na0.31 O22.64 Si7.6'
_chemical_formula_weight     830.64

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
'O' 'O'  0.0106  0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'O2-' 'O2-'  0.0106  0.0060
'Hovesteydt, 1982'
'O-' 'O-'  0.0106  0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'F-' 'F-'  0.0140  0.0100
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Al' 'Al'  0.0645  0.0514
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Si' 'Si'  0.0817  0.0704
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Al3+' 'Al3+'  0.0645  0.0520
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Si4+' 'Si4+'  0.0817  0.0710
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Fe2+' 'Fe2+'  0.3460  0.8450
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Mg2+' 'Mg2+'  0.0490  0.0360
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Fe3+' 'Fe3+'  0.3460  0.8450
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Ca2+' 'Ca2+'  0.2260  0.3060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Na+' 'Na+'  0.0360  0.0250
'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'

_space_group_crystal_system      monoclinic
_space_group_IT_number          12
_space_group_name_H-M_alt       'C 2/m'
_space_group_name_Hall          '-C 2y'

loop_
_space_group_symop_operation_xyz
'x, y, z'
'x, -y, z'

```

fluoro-tremolite 1082\_751\_361.cif

```

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

_cell_length_a          9.8464(17)
_cell_length_b          18.050(3)
_cell_length_c          5.2769(14)
_cell_angle_alpha        90
_cell_angle_beta         104.800(18)
_cell_angle_gamma        90
_cell_volume             906.7(3)
_cell_formula_units_Z    2
_cell_measurement_temperature 298(2)
_cell_measurement_reflns_used 60
_cell_measurement_theta_min 2
_cell_measurement_theta_max 30

_exptl_crystal_description      'prism'
_exptl_crystal_colour           'colourless'
_exptl_crystal_density_meas     ?
_exptl_crystal_density_method   ?
_exptl_crystal_density_diffrn   3.043
_exptl_crystal_F_000            826.2
_exptl_crystal_size_max          0.400
_exptl_crystal_size_mid          0.230
_exptl_crystal_size_min          0.130
_exptl_absorpt_coefficient_mu   1.659
_exptl_absorpt_correction_type   psi-scan
_exptl_absorpt_correction_T_min  0.792
_exptl_absorpt_correction_T_max  0.892
_exptl_absorpt_process_details   ;

North A.C.T., Phillips D.C. & Mathews F.S. (1968) Acta. Cryst. A24, 351
; _exptl_absorpt_special_details   ?

_diffrn_ambient_temperature    298(2)
_diffrn_radiation_wavelength   0.7107
_diffrn_radiation_type          MoK\alpha
_diffrn_radiation_source        'fine-focus sealed tube'
_diffrn_radiation_monochromator graphite
_diffrn_measurement_device_type PHILIPS PW1100
_diffrn_measurement_method      'omega-2theta scans'
_diffrn_standards_number        3
_diffrn_standards_interval_count 400
_diffrn_standards_decay_%       0
_diffrn_reflns_number           2702
_diffrn_reflns_av_R_equivalents 0.012
_diffrn_reflns_limit_h_min      -13
_diffrn_reflns_limit_h_max      13
_diffrn_reflns_limit_k_min      -25
_diffrn_reflns_limit_k_max      25
_diffrn_reflns_limit_l_min      0
_diffrn_reflns_limit_l_max      7
_diffrn_reflns_theta_min        2.257
_diffrn_reflns_theta_max        30.038
_diffrn_measured_fraction_theta_max 0.999
_reflns_number_total           1373
_reflns_number_gt               1229
_reflns_threshold_expression    'I > 3\s(I)'

_computing_data_collection      'local program'
_computing_cell_refinement       'LAT routine of PW1100 diffractometer'
_computing_data_reduction        'local program'
_computing_structure_refinement ORFLS (Busing et al., 1962), modified

_refine_special_details
;
Refinement of F against reflections with F > 3sigma(F).
The threshold expression (_gt) of F > 3sigma(F) corresponds to the cutoff used
to discriminate between observed and unobserved reflections for refinement.
The use of unitary weight produces unusual values for the calculated
weighted WR-factor (similar to R).
;

_refine_ls_structure_factor_coef F
_refine_ls_matrix_type          full
_refine_ls_weighting_scheme      unit
_refine_ls_hydrogen_treatment    mixed
_refine_ls_extinction_method     'secondary isotropic'
_refine_ls_extinction_coef       0.000274(3)
_refine_ls_extinction_expression 'Zachariasen, 1967'
_refine_ls_number_reflns          1229
_refine_ls_number_parameters     134
_refine_ls_number_restraints      0
_refine_ls_R_factor_all           0.0166
_refine_ls_R_factor_gt            0.0130
_refine_ls_wR_factor_ref          0.0172
_refine_ls_wR_factor_gt            0.0136
_refine_ls_restrained_S_all      0.724

loop_
_atom_site_label

```

fluoro-tremolite 1082\_751\_361.cif

```

_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
O1A O 0.11158(7) 0.08528(4) 0.21841(14) 0.0063(2) Uani 0.14(6) 1 d . . P . .
O1B O2- 0.11158(7) 0.08528(4) 0.21841(14) 0.0063(2) Uani 0.86(6) 1 d . . P . .
O2A O 0.11900(7) 0.17061(4) 0.72473(14) 0.0065(2) Uani 0.39(6) 1 d . . P . .
O2B O2- 0.11900(7) 0.17061(4) 0.72473(14) 0.0065(2) Uani 0.61(6) 1 d . . P . .
O3A O- 0.10575(10) 0.0000 0.7142(2) 0.0093(2) Uani 0.32(2) 2 d S T P . .
O3B F- 0.10575(10) 0.0000 0.7142(2) 0.0093(2) Uani 0.68(2) 2 d S T P . .
O4A O 0.36471(8) 0.24827(4) 0.79183(14) 0.0086(2) Uani 0.48(6) 1 d . . P . .
O4B O2- 0.36471(8) 0.24827(4) 0.79183(14) 0.0086(2) Uani 0.52(6) 1 d . . P . .
O5A O 0.34727(8) 0.13502(4) 0.10136(14) 0.0089(2) Uani 0.41(7) 1 d . . P . .
O5B O2- 0.34727(8) 0.13502(4) 0.10136(14) 0.0089(2) Uani 0.59(7) 1 d . . P . .
O6A O 0.34476(8) 0.11829(4) 0.59230(14) 0.0085(2) Uani 0.38(7) 1 d . . P . .
O6B O2- 0.34476(8) 0.11829(4) 0.59230(14) 0.0085(2) Uani 0.62(7) 1 d . . P . .
O7A O 0.33989(11) 0.0000 0.2908(2) 0.0100(3) Uani 0.23(5) 2 d S T P . .
O7B O2- 0.33989(11) 0.0000 0.2908(2) 0.0100(3) Uani 0.77(5) 2 d S T P . .
T1A Al 0.28110(3) 0.08396(2) 0.29806(5) 0.0045(2) Uani 0.07(5) 1 d . . P . .
T1B Si 0.28110(3) 0.08396(2) 0.29806(5) 0.0045(2) Uani 0.64(5) 1 d . . P . .
T1C Al3+ 0.28110(3) 0.08396(2) 0.29806(5) 0.0045(2) Uani 0.03(5) 1 d . . P . .
T1D Si4+ 0.28110(3) 0.08396(2) 0.29806(5) 0.0045(2) Uani 0.26(5) 1 d . . P . .
T2A Si 0.28889(3) 0.17117(2) 0.80540(5) 0.0048(2) Uani 0.57(5) 1 d . . P . .
T2B Si4+ 0.28889(3) 0.17117(2) 0.80540(5) 0.0048(2) Uani 0.43(5) 1 d . . P . .
M1A Fe2+ 0.0000 0.08816(3) 0.5000 0.0062(2) Uani 0.037(2) 2 d S T P . .
M1B Mg2+ 0.0000 0.08816(3) 0.5000 0.0062(2) Uani 0.963(2) 2 d S T P . .
M2A Fe3+ 0.0000 0.17652(2) 0.0000 0.0058(2) Uani 0.080(2) 2 d S T P . .
M2B Mg2+ 0.0000 0.17652(2) 0.0000 0.0058(2) Uani 0.920(2) 2 d S T P . .
M3A Fe2+ 0.0000 0.0000 0.0000 0.0061(2) Uani 0.030(2) 4 d S T P . .
M3B Mg2+ 0.0000 0.0000 0.0000 0.0061(2) Uani 0.970(2) 4 d S T P . .
M4 Ca2+ 0.0000 0.27804(2) 0.5000 0.0089(2) Uani 0.975(2) 2 d S T P . .
A Na+ 0.0000 0.5000 0.0000 0.021(6) Uani 0.064(2) 4 d S T P . .
AM Na+ 0.0451(14) 0.5000 0.104(3) 0.027(4) Uani 0.085(3) 2 d S T P . .
A2 Na+ 0.0000 0.4721(11) 0.0000 0.025(9) Uani 0.036(3) 2 d S T P . .
H H 0.195(5) 0.0000 0.762(9) 0.013 Uiso 0.49(4) 2 d S . P . .
M42 Mg2+ 0.0000 0.2616(7) 0.5000 0.010(2) Uiso 0.046(2) 2 d S . P . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
01A 0.0058(3) 0.0064(3) 0.0066(3) -0.0004(3) 0.0017(2) -0.0004(2)
01B 0.0058(3) 0.0064(3) 0.0066(3) -0.0004(3) 0.0017(2) -0.0004(2)
02A 0.0055(3) 0.0076(3) 0.0066(3) -0.0005(3) 0.0018(2) -0.0001(2)
02B 0.0055(3) 0.0076(3) 0.0066(3) -0.0005(3) 0.0018(2) -0.0001(2)
03A 0.0105(4) 0.0089(3) 0.0086(4) 0.0000 0.0026(3) 0.0000
03B 0.0105(4) 0.0089(3) 0.0086(4) 0.0000 0.0026(3) 0.0000
04A 0.0102(3) 0.0069(3) 0.0089(3) -0.0029(3) 0.0032(3) -0.0009(3)
04B 0.0102(3) 0.0069(3) 0.0089(3) -0.0029(3) 0.0032(3) -0.0009(3)
05A 0.0076(3) 0.0109(3) 0.0080(3) 0.0000(3) 0.0016(3) 0.0032(3)
05B 0.0076(3) 0.0109(3) 0.0080(3) 0.0000(3) 0.0016(3) 0.0032(3)
06A 0.0074(3) 0.0102(3) 0.0079(3) 0.0003(3) 0.0019(3) -0.0028(3)
06B 0.0074(3) 0.0102(3) 0.0079(3) 0.0003(3) 0.0019(3) -0.0028(3)
07A 0.0089(5) 0.0068(5) 0.0140(5) 0.0000 0.0026(4) 0.0000
07B 0.0089(5) 0.0068(5) 0.0140(5) 0.0000 0.0026(4) 0.0000
T1A 0.00450(14) 0.0043(2) 0.00476(12) -0.00044(9) 0.00111(10) -0.00033(9)
T1B 0.00450(14) 0.0043(2) 0.00476(12) -0.00044(9) 0.00111(10) -0.00033(9)
T1C 0.00450(14) 0.0043(2) 0.00476(12) -0.00044(9) 0.00111(10) -0.00033(9)
T1D 0.00450(14) 0.0043(2) 0.00476(12) -0.00044(9) 0.00111(10) -0.00033(9)
T2A 0.00468(14) 0.0051(2) 0.00456(12) -0.00078(9) 0.00135(10) -0.00005(9)
T2B 0.00468(14) 0.0051(2) 0.00456(12) -0.00078(9) 0.00135(10) -0.00005(9)
M1A 0.0070(2) 0.0059(2) 0.0060(2) 0.0000 0.0023(2) 0.0000
M1B 0.0070(2) 0.0059(2) 0.0060(2) 0.0000 0.0023(2) 0.0000
M2A 0.0062(2) 0.0054(2) 0.0060(2) 0.0000 0.0020(2) 0.0000
M2B 0.0062(2) 0.0054(2) 0.0060(2) 0.0000 0.0020(2) 0.0000
M3A 0.0070(4) 0.0056(3) 0.0056(3) 0.0000 0.0013(2) 0.0000
M3B 0.0070(4) 0.0056(3) 0.0056(3) 0.0000 0.0013(2) 0.0000
M4A 0.01116(14) 0.0069(2) 0.0108(2) 0.0000 0.00691(10) 0.0000
M4B 0.01116(14) 0.0069(2) 0.0108(2) 0.0000 0.00691(10) 0.0000
A 0.024(10) 0.023(10) 0.018(9) 0.0000 0.010(7) 0.0000
AM 0.016(5) 0.047(7) 0.020(6) 0.0000 0.007(5) 0.0000
A2 0.025(12) 0.012(7) 0.05(2) 0.0000 0.033(13) 0.0000

_geom_special_details
;
Geometry data (distances and angles) are reported only for T, M and A
sites flagged by the A suffix.
All esds are estimated using the full covariance matrix.
;

loop_
_geom_bond_atom_site_label_1

```

fluoro-tremolite 1082\_751\_361.cif

```

_geom_bond_atom_site_label_2
_geom_bond_distance
_geom_bond_site_symmetry_2
_geom_bond_publ_flag
T1A O1A 1.6140(8) . ?
T1A O7A 1.6262(5) . ?
T1A O6A 1.6403(9) . ?
T1A O5A 1.6422(8) . ?
T2A O4A 1.5895(8) . ?
T2A O2A 1.6173(8) . ?
T2A O5A 1.6543(8) 1_556 ?
T2A O6A 1.6716(8) . ?
M1A O1A 2.0620(8) . ?
M1A O1A 2.0620(8) 6_556 ?
M1A O2A 2.0698(8) . ?
M1A O2A 2.0698(8) 6_556 ?
M1A O3A 2.0720(7) . ?
M1A O3A 2.0720(7) 5_556 ?
M2A O4A 2.0191(8) 7_556 ?
M2A O4A 2.0191(8) 4_454 ?
M2A O2A 2.0890(8) 6_556 ?
M2A O2A 2.0890(8) 1_554 ?
M2A O1A 2.1449(9) 6 ?
M2A O1A 2.1449(9) . ?
M3A O3A 2.0397(10) 5_556 ?
M3A O3A 2.0397(10) 1_554 ?
M3A O1A 2.0634(7) . ?
M3A O1A 2.0634(7) 5 ?
M3A O1A 2.0634(7) 2 ?
M3A O1A 2.0634(7) 6 ?
M4 O4A 2.3280(9) 4_455 ?
M4 O4A 2.3280(9) 7_556 ?
M4 O2A 2.4144(9) . ?
M4 O2A 2.4144(9) 6_556 ?
M4 O6A 2.5408(8) 7_556 ?
M4 O6A 2.5408(8) 4_455 ?
M4 O5A 2.7447(9) 7_556 ?
M4 O5A 2.7447(9) 4_455 ?
A O7A 2.4649(12) 7 ?
A O7A 2.4649(12) 3_455 ?
A O5A 2.9829(9) 8 ?
A O5A 2.9829(9) 4_455 ?
A O5A 2.9829(9) 7 ?
A O5A 2.9829(9) 3_455 ?
A O6A 3.1374(9) 8_556 ?
A O6A 3.1374(9) 4_454 ?
A O6A 3.1374(9) 7_556 ?
A O6A 3.1374(9) 3_454 ?
AM O7A 2.464(13) 3_455 ?
AM O7A 2.613(13) 7 ?
AM O6A 2.724(8) 8_556 ?
AM O6A 2.724(8) 7_556 ?
AM O5A 2.970(8) 7 ?
AM O5A 2.970(8) 8 ?
AM O7A 3.105(14) 7_556 ?
AM O5A 3.118(8) 4_455 ?
AM O5A 3.118(8) 3_455 ?
A2 O7A 2.516(4) 3_455 ?
A2 O7A 2.516(4) 7 ?
A2 O5A 2.59(2) 4_455 ?
A2 O5A 2.59(2) 7 ?
A2 O6A 2.819(12) 4_454 ?
A2 O6A 2.819(12) 7_556 ?
M42 O2A 2.183(9) . ?
M42 O2A 2.183(9) 6_556 ?
M42 O4A 2.286(13) 4_455 ?
M42 O4A 2.286(13) 7_556 ?
M42 O6A 2.767(9) 7_556 ?
M42 O6A 2.767(9) 4_455 ?
M42 O5A 2.925(8) 7_556 ?
M42 O5A 2.925(8) 4_455 ?
O3A H 0.85(5) . ?

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
O1A T1A O7A 110.99(5) . . ?
O1A T1A O6A 111.14(4) . . ?
O7A T1A O6A 108.79(5) . . ?
O1A T1A O5A 112.21(4) . . ?
O7A T1A O5A 107.88(5) . . ?
O6A T1A O5A 105.60(4) . . ?
O4A T2A O2A 117.37(4) . . ?
O4A T2A O5A 109.50(4) . 1_556 ?
O2A T2A O5A 109.43(4) . 1_556 ?
O4A T2A O6A 103.32(4) . . ?
O2A T2A O6A 108.39(4) . . ?
O5A T2A O6A 108.37(4) 1_556 ?
O1A M1A O1A 177.11(5) . 6_556 ?
O1A M1A O2A 95.92(3) . . ?
O1A M1A O2A 86.16(3) 6_556 . ?

```

01A M1A O2A 86.16(3) . 6\_556 ?  
 01A M1A O2A 95.92(3) 6\_556 6\_556 ?  
 02A M1A O2A 88.06(5) . 6\_556 ?  
 01A M1A O3A 95.04(4) . . ?  
 01A M1A O3A 82.73(4) 6\_556 . ?  
 02A M1A O3A 96.17(3) . . ?  
 02A M1A O3A 175.45(4) 6\_556 . ?  
 01A M1A O3A 82.73(4) . 5\_556 ?  
 01A M1A O3A 95.04(4) 6\_556 5\_556 ?  
 02A M1A O3A 175.45(4) . 5\_556 ?  
 02A M1A O3A 96.17(3) 6\_556 5\_556 ?  
 03A M1A O3A 79.65(5) . 5\_556 ?  
 04A M2A O4A 95.50(5) 7\_556 4\_454 ?  
 04A M2A O2A 93.75(3) 7\_556 6\_556 ?  
 04A M2A O2A 90.19(3) 4\_454 6\_556 ?  
 04A M2A O2A 90.19(3) 7\_556 1\_554 ?  
 04A M2A O2A 93.75(3) 4\_454 1\_554 ?  
 02A M2A O2A 174.14(5) 6\_556 1\_554 ?  
 04A M2A O1A 169.99(3) 7\_556 6 ?  
 04A M2A O1A 92.73(3) 4\_454 6 ?  
 02A M2A O1A 91.90(3) 6\_556 6 ?  
 02A M2A O1A 83.60(3) 1\_554 6 ?  
 04A M2A O1A 92.73(3) 7\_556 . ?  
 04A M2A O1A 169.99(3) 4\_454 . ?  
 02A M2A O1A 83.60(3) 6\_556 . ?  
 02A M2A O1A 91.90(3) 1\_554 . ?  
 01A M2A O1A 79.69(4) 6 . ?  
 03A M3A O3A 180.0 5\_556 1\_554 ?  
 03A M3A O1A 83.49(3) 5\_556 . ?  
 03A M3A O1A 96.51(3) 1\_554 . ?  
 03A M3A O1A 96.51(3) 5\_556 5 ?  
 03A M3A O1A 83.49(3) 1\_554 5 ?  
 01A M3A O1A 180.0 . 5 ?  
 03A M3A O1A 83.49(3) 5\_556 2 ?  
 03A M3A O1A 96.51(3) 1\_554 2 ?  
 01A M3A O1A 96.49(3) . 2 ?  
 01A M3A O1A 83.51(3) 5 2 ?  
 03A M3A O1A 96.51(3) 5\_556 6 ?  
 03A M3A O1A 83.49(3) 1\_554 6 ?  
 01A M3A O1A 83.51(3) . 6 ?  
 01A M3A O1A 96.49(3) 5 6 ?  
 01A M3A O1A 180.0 2 6 ?  
 04A M4 O4A 156.46(4) 4\_455 7\_556 ?  
 04A M4 O2A 78.42(3) 4\_455 . ?  
 04A M4 O2A 82.71(3) 7\_556 . ?  
 04A M4 O2A 82.71(3) 4\_455 6\_556 ?  
 04A M4 O2A 78.42(3) 7\_556 6\_556 ?  
 02A M4 O2A 73.14(4) . 6\_556 ?  
 04A M4 O6A 138.67(3) 4\_455 7\_556 ?  
 04A M4 O6A 63.22(3) 7\_556 7\_556 ?  
 02A M4 O6A 116.45(3) . 7\_556 ?  
 02A M4 O6A 137.53(3) 6\_556 7\_556 ?  
 04A M4 O6A 63.22(3) 4\_455 4\_455 ?  
 04A M4 O6A 138.67(3) 7\_556 4\_455 ?  
 02A M4 O6A 137.53(3) . 4\_455 ?  
 02A M4 O6A 116.45(3) 6\_556 4\_455 ?  
 06A M4 O6A 85.14(4) 7\_556 4\_455 ?  
 04A M4 O5A 84.48(3) 4\_455 7\_556 ?  
 04A M4 O5A 109.24(3) 7\_556 7\_556 ?  
 02A M4 O5A 88.89(3) . 7\_556 ?  
 02A M4 O5A 159.68(2) 6\_556 7\_556 ?  
 06A M4 O5A 59.15(3) 7\_556 7\_556 ?  
 06A M4 O5A 70.77(3) 4\_455 7\_556 ?  
 04A M4 O5A 109.24(3) 4\_455 4\_455 ?  
 04A M4 O5A 84.48(3) 7\_556 4\_455 ?  
 02A M4 O5A 159.68(2) . 4\_455 ?  
 02A M4 O5A 88.89(3) 6\_556 4\_455 ?  
 06A M4 O5A 70.77(3) 7\_556 4\_455 ?  
 06A M4 O5A 59.15(3) 4\_455 4\_455 ?  
 05A M4 O5A 110.25(4) 7\_556 4\_455 ?  
 07A A 07A 180.0 7 3\_455 ?  
 07A A 05A 57.07(2) 7 ?  
 07A A 05A 122.93(2) 3\_455 8 ?  
 07A A 05A 122.93(2) 7 4\_455 ?  
 07A A 05A 57.07(2) 3\_455 4\_455 ?  
 05A A 05A 180.0 8 4\_455 ?  
 07A A 05A 57.07(2) 7 7 ?  
 07A A 05A 122.93(2) 3\_455 7 ?  
 05A A 05A 189.57(3) 8 7 ?  
 05A A 05A 70.43(3) 4\_455 7 ?  
 07A A 05A 122.93(2) 7 3\_455 ?  
 07A A 05A 57.07(2) 3\_455 3\_455 ?  
 05A A 05A 70.43(3) 8 3\_455 ?  
 05A A 05A 189.57(3) 4\_455 3\_455 ?  
 05A A 05A 180.0 7 3\_455 ?  
 07A A 06A 98.62(3) 7 8\_556 ?  
 07A A 06A 81.38(3) 3\_455 8\_556 ?  
 05A A 06A 52.22(2) 8 8\_556 ?  
 05A A 06A 127.78(2) 4\_455 8\_556 ?  
 05A A 06A 119.95(2) 7 8\_556 ?  
 05A A 06A 60.05(2) 3\_455 8\_556 ?  
 07A A 06A 81.38(3) 7 4\_454 ?  
 07A A 06A 98.62(3) 3\_455 4\_454 ?  
 05A A 06A 127.78(2) 8 4\_454 ?  
 05A A 06A 52.22(2) 4\_455 4\_454 ?  
 05A A 06A 60.05(2) 7 4\_454 ?

05A A 06A 119.95(2) 3\_455 4\_454 ?  
 06A A 06A 180.0 8\_556 4\_454 ?  
 07A A 06A 98.62(3) 7\_556 ?  
 07A A 06A 81.38(3) 3\_455 7\_556 ?  
 05A A 06A 119.95(2) 8\_7\_556 ?  
 05A A 06A 60.05(2) 4\_455 7\_556 ?  
 05A A 06A 52.22(2) 7\_7\_556 ?  
 05A A 06A 127.78(2) 3\_455 7\_556 ?  
 06A A 06A 85.77(3) 8\_556 7\_556 ?  
 06A A 06A 94.23(3) 4\_454 7\_556 ?  
 07A A 06A 81.38(3) 7\_3\_454 ?  
 07A A 06A 98.62(3) 3\_455 3\_454 ?  
 05A A 06A 60.05(2) 8\_3\_454 ?  
 05A A 06A 119.95(2) 4\_455 3\_454 ?  
 05A A 06A 127.78(2) 7\_3\_454 ?  
 05A A 06A 52.22(2) 3\_455 3\_454 ?  
 06A A 06A 94.23(3) 8\_556 3\_454 ?  
 06A A 06A 85.77(3) 4\_454 3\_454 ?  
 06A A 06A 180.0 7\_556 3\_454 ?  
 07A AM 07A 152.4(6) 3\_455 7 ?  
 07A AM 06A 90.5(3) 3\_455 8\_556 ?  
 07A AM 06A 106.3(3) 7\_8\_556 ?  
 07A AM 06A 90.5(3) 3\_455 7\_556 ?  
 07A AM 06A 106.3(3) 7\_7\_556 ?  
 06A AM 06A 103.2(5) 8\_556 7\_556 ?  
 07A AM 05A 123.5(2) 3\_455 7 ?  
 07A AM 05A 56.1(2) 7\_7 ?  
 06A AM 05A 137.1(5) 8\_556 7 ?  
 06A AM 05A 56.35(10) 7\_556 7 ?  
 07A AM 05A 123.5(2) 3\_455 8 ?  
 07A AM 05A 56.1(2) 7\_8 ?  
 06A AM 05A 56.35(10) 8\_556 8 ?  
 06A AM 05A 137.1(5) 7\_556 8 ?  
 05A AM 05A 110.3(4) 7\_8 ?  
 07A AM 07A 73.1(3) 3\_455 7\_556 ?  
 07A AM 07A 134.6(5) 7\_7\_556 ?  
 06A AM 07A 53.7(3) 8\_556 7\_556 ?  
 06A AM 07A 53.7(3) 7\_556 7\_556 ?  
 05A AM 07A 107.7(3) 7\_7\_556 ?  
 05A AM 07A 107.7(3) 8\_7\_556 ?  
 07A AM 05A 55.0(2) 3\_455 4\_455 ?  
 07A AM 05A 113.2(3) 7\_4\_455 ?  
 06A AM 05A 140.3(5) 8\_556 4\_455 ?  
 06A AM 05A 62.88(10) 7\_556 4\_455 ?  
 05A AM 05A 68.77(8) 7\_4\_455 ?  
 05A AM 05A 157.0(5) 8\_4\_455 ?  
 07A AM 05A 93.9(3) 7\_556 4\_455 ?  
 07A AM 05A 55.0(2) 3\_455 3\_455 ?  
 07A AM 05A 113.2(3) 7\_3\_455 ?  
 06A AM 05A 62.88(10) 8\_556 3\_455 ?  
 06A AM 05A 140.3(5) 7\_556 3\_455 ?  
 05A AM 05A 157.0(5) 7\_3\_455 ?  
 05A AM 05A 68.77(8) 8\_3\_455 ?  
 07A AM 05A 93.9(3) 7\_556 3\_455 ?  
 05A AM 05A 102.8(4) 4\_455 3\_455 ?  
 07A A2 07A 156.9(9) 3\_455 7 ?  
 07A A2 05A 62.3(2) 3\_455 4\_455 ?  
 07A A2 05A 139.8(7) 7\_4\_455 ?  
 07A A2 05A 139.8(7) 3\_455 7 ?  
 07A A2 05A 62.3(2) 7\_7 ?  
 05A A2 05A 83.3(6) 4\_455 7 ?  
 07A A2 06A 106.2(2) 3\_455 4\_454 ?  
 07A A2 06A 87.3(2) 7\_4\_454 ?  
 05A A2 06A 59.7(3) 4\_455 4\_454 ?  
 05A A2 06A 68.9(4) 7\_4\_454 ?  
 07A A2 06A 87.3(2) 3\_455 7\_556 ?  
 07A A2 06A 106.2(2) 7\_7\_556 ?  
 05A A2 06A 68.9(4) 4\_455 7\_556 ?  
 05A A2 06A 59.7(3) 7\_7\_556 ?  
 06A A2 06A 109.3(7) 4\_454 7\_556 ?  
 02A M42 02A 82.4(4) . 6\_556 ?  
 02A M42 04A 84.3(2) . 4\_455 ?  
 02A M42 04A 89.0(2) 6\_556 4\_455 ?  
 02A M42 04A 89.0(2) . 7\_556 ?  
 02A M42 04A 84.3(2) 6\_556 7\_556 ?  
 04A M42 04A 171.1(6) 4\_455 7\_556 ?  
 02A M42 06A 116.17(5) . 7\_556 ?  
 02A M42 06A 137.55(5) 6\_556 7\_556 ?  
 04A M42 06A 128.5(4) 4\_455 7\_556 ?  
 04A M42 06A 59.9(2) 7\_556 7\_556 ?  
 02A M42 06A 137.55(5) . 4\_455 ?  
 02A M42 06A 116.17(5) 6\_556 4\_455 ?  
 04A M42 06A 59.9(2) 4\_455 4\_455 ?  
 04A M42 06A 128.5(4) 7\_556 4\_455 ?  
 06A M42 06A 76.8(3) 7\_556 4\_455 ?  
 02A M42 05A 89.04(4) . 7\_556 ?  
 02A M42 05A 167.6(3) 6\_556 7\_556 ?  
 04A M42 05A 81.2(2) 4\_455 7\_556 ?  
 04A M42 05A 104.7(2) 7\_556 7\_556 ?  
 06A M42 05A 54.6(2) 7\_556 7\_556 ?  
 06A M42 05A 65.1(2) 4\_455 7\_556 ?  
 02A M42 05A 167.6(3) . 4\_455 ?  
 02A M42 05A 89.04(4) 6\_556 4\_455 ?  
 04A M42 05A 104.7(2) 4\_455 4\_455 ?  
 04A M42 05A 81.2(2) 7\_556 4\_455 ?  
 06A M42 05A 65.1(2) 7\_556 4\_455 ?

fluoro-tremolite 1082\_751\_361.cif

06A M42 05A 54.6(2) 4\_455 4\_455 ?  
 05A M42 05A 100.7(4) 7\_556 4\_455 ?  
 T1A 05A T2A 136.03(5) . 1\_554 ?  
 T1A 06A T2A 137.78(5) . . ?  
 T1A 07A T1A 137.47(7) . 2 ?  
 05A 06A 05A 166.90(5) . 1\_556 ?  
 06A 07A 06A 107.01(5) 2 . ?  
 \_refine\_diff\_density\_max 0.35  
 \_refine\_diff\_density\_min -0.18

loop\_  
 \_refln\_index\_h  
 \_refln\_index\_k  
 \_refln\_index\_l  
 \_refln\_F\_squared\_meas  
 \_refln\_F\_squared\_sigma  
 0 2 0 788.5 3.5  
 0 4 0 3178.0 10.0  
 0 6 0 0.1 1.2  
 0 8 0 276.2 4.5  
 0 10 0 2678.6 15.0  
 0 12 0 17829.1 42.6  
 0 14 0 5.1 2.4  
 0 16 0 55.5 3.9  
 0 18 0 192.3 6.3  
 0 20 0 2957.4 24.5  
 0 22 0 3145.9 27.1  
 0 24 0 5119.1 36.9  
 1 1 0 1350.8 16.1  
 1 3 0 614.4 3.0  
 1 5 0 11.0 1.1  
 1 7 0 17.5 1.3  
 1 9 0 2906.2 16.0  
 1 11 0 9180.7 20.7  
 1 13 0 71.6 16.6  
 1 15 0 30.9 2.2  
 1 17 0 4.6 3.0  
 1 19 0 14.1 2.7  
 1 21 0 370.2 8.2  
 1 23 0 139.1 10.9  
 1 25 0 126.1 7.4  
 2 0 0 319.5 3.4  
 2 2 0 603.3 6.2  
 2 4 0 5776.6 93.3  
 2 6 0 25.0 2.2  
 2 8 0 218.5 3.9  
 2 10 0 564.6 5.2  
 2 12 0 942.1 7.4  
 2 14 0 435.6 8.9  
 2 16 0 53.1 2.7  
 2 18 0 572.7 9.3  
 2 20 0 119.3 4.4  
 2 22 0 319.8 13.9  
 2 24 0 920.6 11.6  
 3 1 0 8963.0 42.3  
 3 3 0 2419.1 12.0  
 3 5 0 2346.1 11.0  
 3 7 0 3209.7 40.6  
 3 9 0 282.8 3.8  
 3 11 0 4635.5 15.8  
 3 13 0 2.2 1.7  
 3 15 0 12.4 2.7  
 3 17 0 248.6 5.1  
 3 19 0 578.3 11.4  
 3 21 0 47.1 6.5  
 3 23 0 890.8 11.3  
 4 0 0 48.6 2.5  
 4 2 0 202.8 12.8  
 4 4 0 64.6 1.9  
 4 6 0 124.1 18.3  
 4 8 0 5546.5 32.3  
 4 10 0 1401.8 29.9  
 4 12 0 1043.7 8.4  
 4 14 0 100.2 3.3  
 4 16 0 2423.2 14.6  
 4 18 0 228.9 5.3  
 4 20 0 1469.4 21.4  
 4 22 0 1171.4 12.6  
 4 24 0 7.8 5.9  
 5 1 0 4573.3 16.5  
 5 3 0 2382.8 12.5  
 5 5 0 159.1 4.7  
 5 7 0 869.5 6.9  
 5 9 0 16.5 1.8  
 5 11 0 411.8 5.5  
 5 13 0 2276.5 13.3  
 5 15 0 885.1 25.6  
 5 17 0 5.2 3.2  
 5 19 0 54.8 3.6  
 5 21 0 933.6 16.7  
 5 23 0 1667.9 71.9  
 6 0 0 6969.3 26.9  
 6 2 0 1044.8 7.6  
 6 4 0 38.6 2.0  
 6 6 0 85.9 3.0

## fluoro-tremolite 1082\_751\_361.cif

6	8	0	1497.9	10.7
6	10	0	71.6	2.8
6	12	0	190.7	4.4
6	14	0	30.6	6.0
6	16	0	89.2	3.8
6	18	0	543.7	10.8
6	20	0	127.7	5.0
6	22	0	307.4	13.8
7	1	0	2967.7	14.5
7	3	0	885.3	30.1
7	5	0	82.6	2.9
7	7	0	447.3	5.9
7	9	0	5505.5	20.6
7	11	0	11921.0	141.8
7	13	0	870.3	9.3
7	15	0	1499.5	12.7
7	17	0	29.2	7.0
7	19	0	520.2	10.6
7	21	0	36.7	4.1
8	0	0	6732.0	31.5
8	2	0	336.6	10.7
8	4	0	238.1	7.1
8	6	0	398.4	6.1
8	8	0	28.0	2.9
8	10	0	279.1	5.7
8	12	0	931.2	23.3
8	14	0	33.1	3.2
8	16	0	56.9	3.7
8	18	0	3.2	3.2
8	20	0	95.6	4.9
9	1	0	382.5	8.5
9	3	0	208.5	4.7
9	5	0	6.7	3.6
9	7	0	2169.9	40.0
9	9	0	136.9	4.3
9	11	0	298.9	6.2
9	13	0	302.4	6.6
9	15	0	673.0	9.6
9	17	0	210.9	6.1
10	0	0	4297.6	29.4
10	2	0	100.5	4.0
10	4	0	2.3	3.4
10	6	0	74.8	5.8
10	8	0	2170.8	15.7
10	10	0	590.9	17.3
10	12	0	2937.4	19.3
10	14	0	1.9	2.9
10	16	0	1006.0	12.4
11	1	0	1984.7	15.3
11	3	0	85.1	4.1
11	5	0	518.6	9.2
11	7	0	1.5	3.4
11	9	0	236.1	11.5
11	11	0	2691.9	19.2
11	13	0	160.8	5.9
12	0	0	71.9	6.4
12	2	0	10.3	4.0
12	4	0	318.3	7.1
12	6	0	16.9	5.4
12	8	0	823.1	11.1
12	10	0	241.3	6.8
13	1	0	490.1	9.0
13	3	0	146.4	5.8
13	5	0	77.4	4.7
0	0	1	503.8	3.9
0	2	1	105.0	4.1
0	4	1	41.9	1.3
0	6	1	8151.9	97.0
0	8	1	156.1	2.6
0	10	1	1599.6	8.5
0	12	1	560.3	5.7
0	14	1	952.3	8.0
0	16	1	1989.8	23.2
0	18	1	0.6	3.4
0	20	1	59.2	3.4
0	22	1	16.5	3.2
0	24	1	6.1	6.5
1	1	1	393.1	6.4
-1	1	1	1855.4	5.2
1	3	1	7094.7	203.8
-1	3	1	2272.0	63.0
1	5	1	16563.7	454.2
-1	5	1	1315.4	14.5
1	7	1	1836.7	8.0
-1	7	1	6046.7	13.8
1	9	1	411.8	4.3
-1	9	1	5622.9	53.7
1	11	1	250.8	3.8
-1	11	1	44.9	3.6
1	13	1	823.6	16.2
-1	13	1	1673.1	10.0
1	15	1	2165.0	19.5
-1	15	1	995.8	8.6
1	17	1	9780.0	87.0
-1	17	1	1127.1	10.0
1	19	1	1207.1	27.4

## fluoro-tremolite 1082\_751\_361.cif

-1	19	1	399.4	6.5
1	21	1	2082.6	32.4
-1	21	1	281.2	6.2
1	23	1	45.7	3.6
-1	23	1	327.0	7.0
1	25	1	759.1	12.8
-1	25	1	17.0	3.8
2	0	1	627.0	5.7
-2	0	1	481.7	4.5
2	2	1	7065.6	149.7
-2	2	1	11.6	1.0
2	4	1	71.2	2.5
-2	4	1	159.1	2.2
2	6	1	11056.2	320.7
-2	6	1	1571.5	26.9
2	8	1	6.9	1.5
-2	8	1	6.5	1.3
2	10	1	963.9	14.7
-2	10	1	160.2	3.0
2	12	1	237.3	7.4
-2	12	1	366.9	6.5
2	14	1	383.4	5.4
-2	14	1	3104.0	39.9
2	16	1	1496.4	11.2
-2	16	1	1604.7	42.1
2	18	1	4.8	2.6
-2	18	1	237.7	5.1
2	20	1	176.5	4.9
-2	20	1	84.7	3.9
2	22	1	155.2	5.2
-2	22	1	796.9	10.0
2	24	1	24.2	3.8
-2	24	1	90.7	4.6
3	1	1	350.7	3.6
-3	1	1	506.8	3.8
3	3	1	560.0	4.7
-3	3	1	5780.6	93.3
3	5	1	6495.2	40.6
-3	5	1	9828.1	291.7
3	7	1	16.5	1.6
-3	7	1	558.0	4.8
3	9	1	214.7	3.6
-3	9	1	1159.7	11.7
3	11	1	154.3	6.8
-3	11	1	1448.7	12.8
3	13	1	1169.1	9.2
-3	13	1	6.7	2.6
3	15	1	49.8	2.8
-3	15	1	504.5	8.3
3	17	1	334.0	11.0
-3	17	1	2655.6	15.2
3	19	1	14.0	3.4
-3	19	1	119.6	4.0
3	21	1	5.9	3.4
-3	21	1	385.8	7.1
3	23	1	438.6	19.3
-3	23	1	338.6	15.3
4	0	1	395.7	5.8
-4	0	1	757.2	7.2
4	2	1	815.8	11.1
-4	2	1	5281.5	37.6
4	4	1	3.1	4.7
-4	4	1	157.3	2.6
4	6	1	16020.2	555.8
-4	6	1	1374.0	7.6
4	8	1	203.0	3.6
-4	8	1	12.0	2.1
4	10	1	478.5	12.0
-4	10	1	797.0	10.4
4	12	1	166.5	3.9
-4	12	1	182.7	6.4
4	14	1	5950.0	21.8
-4	14	1	17.1	2.1
4	16	1	3124.4	17.1
-4	16	1	1055.2	9.7
4	18	1	4596.5	21.8
-4	18	1	189.9	11.5
4	20	1	43.6	3.6
-4	20	1	198.1	5.3
4	22	1	888.1	11.2
-4	22	1	3.2	3.8
-4	24	1	33.4	4.0
5	1	1	51.3	2.1
-5	1	1	250.6	5.7
5	3	1	45.5	2.0
-5	3	1	304.0	5.9
5	5	1	4965.2	53.5
-5	5	1	829.1	8.1
5	7	1	333.9	8.1
-5	7	1	1251.8	14.0
5	9	1	413.3	18.3
-5	9	1	1007.6	7.8
5	11	1	370.8	9.5
-5	11	1	21.7	2.0
5	13	1	130.9	3.9
-5	13	1	244.9	4.6

## fluoro-tremolite 1082\_751\_361.cif

5	15	1	97.5	3.7
-5	15	1	25.3	2.9
5	17	1	962.1	10.4
-5	17	1	197.0	4.9
5	19	1	111.6	4.5
-5	19	1	21.9	3.8
5	21	1	0.1	4.3
-5	21	1	108.4	4.7
-5	23	1	108.7	5.2
6	0	1	146.6	4.6
-6	0	1	262.2	5.5
6	2	1	1566.9	13.5
-6	2	1	330.6	9.2
6	4	1	3.1	1.6
-6	4	1	53.6	2.2
6	6	1	3790.7	18.5
-6	6	1	26160.3	1045.6
6	8	1	70.1	2.9
-6	8	1	583.2	6.3
6	10	1	23.6	3.2
-6	10	1	1186.2	9.2
6	12	1	396.9	6.3
-6	12	1	270.1	16.7
6	14	1	201.4	5.0
-6	14	1	1476.1	12.9
6	16	1	342.1	6.5
-6	16	1	2040.2	21.9
6	18	1	5032.7	56.5
-6	18	1	2955.9	36.7
6	20	1	612.1	9.5
-6	20	1	43.6	6.7
6	22	1	3.7	6.9
-6	22	1	-0.4	3.2
7	1	1	43.3	2.4
-7	1	1	8.8	2.0
7	3	1	816.2	7.9
-7	3	1	505.5	5.8
7	5	1	684.6	10.1
-7	5	1	10278.1	44.7
7	7	1	363.8	15.1
-7	7	1	1519.9	19.6
7	9	1	32.8	2.6
-7	9	1	76.9	3.0
7	11	1	4.2	2.6
-7	11	1	98.1	3.4
7	13	1	12.2	2.9
-7	13	1	11.7	2.9
7	15	1	426.1	10.3
-7	15	1	97.1	3.9
7	17	1	587.5	8.9
-7	17	1	4623.3	68.0
7	19	1	29.0	17.4
-7	19	1	798.1	10.4
-7	21	1	295.6	7.0
8	0	1	275.4	7.1
-8	0	1	93.7	4.3
8	2	1	101.9	3.7
-8	2	1	1247.1	12.6
8	4	1	24.2	2.6
-8	4	1	4.5	2.0
8	6	1	6783.6	24.4
-8	6	1	581.9	7.0
8	8	1	78.8	7.8
-8	8	1	124.8	3.7
8	10	1	459.7	18.3
-8	10	1	118.2	3.9
8	12	1	30.4	4.7
-8	12	1	212.2	5.0
8	14	1	775.0	14.9
-8	14	1	8.1	2.9
8	16	1	1068.2	12.0
-8	16	1	823.3	10.2
8	18	1	413.5	8.2
-8	18	1	1248.9	21.9
-8	20	1	362.0	7.8
9	1	1	4.9	6.4
-9	1	1	120.1	3.8
9	3	1	7.2	2.6
-9	3	1	379.3	6.0
9	5	1	66.2	3.4
-9	5	1	1932.0	14.1
9	7	1	628.9	8.3
-9	7	1	5.2	2.7
9	9	1	423.4	7.2
-9	9	1	7.4	3.0
9	11	1	236.9	5.8
-9	11	1	63.6	6.3
9	13	1	171.4	5.3
-9	13	1	432.2	7.5
9	15	1	33.7	3.9
-9	15	1	0.6	3.3
9	17	1	38.3	3.9
-9	17	1	113.9	7.6
-9	19	1	3.5	3.5
10	0	1	4.0	4.4
-10	0	1	122.5	5.7

## fluoro-tremolite 1082\_751\_361.cif

10	2	1	598.7	8.5
-10	2	1	155.5	4.5
10	4	1	418.4	7.4
-10	4	1	55.2	3.3
10	6	1	275.9	9.4
-10	6	1	3741.5	19.6
10	8	1	268.0	6.3
-10	8	1	2.0	3.3
10	10	1	256.8	6.3
-10	10	1	220.6	5.5
10	12	1	177.6	5.5
-10	12	1	113.7	18.7
10	14	1	110.0	5.0
-10	14	1	1939.7	16.1
-10	16	1	1574.1	23.8
11	1	1	11.3	3.4
-11	1	1	5.7	2.9
11	3	1	1424.7	33.5
-11	3	1	22.0	3.1
11	5	1	6064.8	75.7
-11	5	1	51.1	9.3
11	7	1	1504.6	14.5
-11	7	1	951.9	22.3
11	9	1	346.7	9.3
-11	9	1	679.8	9.5
11	11	1	38.5	5.2
-11	11	1	320.0	15.2
-11	13	1	28.5	4.1
-11	15	1	29.8	3.9
12	0	1	403.3	11.4
-12	0	1	51.5	5.5
12	2	1	20.4	3.9
-12	2	1	993.0	11.5
12	4	1	125.2	5.2
-12	4	1	434.8	8.0
12	6	1	1597.8	21.1
-12	6	1	23.6	3.8
12	8	1	27.8	6.2
-12	8	1	232.1	8.0
-12	10	1	88.5	4.6
-12	12	1	169.3	8.2
-13	1	1	20.3	3.7
-13	3	1	984.8	24.0
-13	5	1	2510.6	23.5
-13	7	1	144.6	5.6
0	0	2	4719.8	16.6
0	2	2	609.2	9.3
0	4	2	94.7	2.1
0	6	2	16.4	1.4
0	8	2	788.2	13.0
0	10	2	136.0	3.8
0	12	2	8050.1	98.1
0	14	2	464.8	6.0
0	16	2	46.5	2.8
0	18	2	495.7	7.3
0	20	2	8.1	2.6
0	22	2	134.6	4.9
0	24	2	2036.2	42.7
1	1	2	22.1	2.4
-1	1	2	35.8	7.4
1	3	2	516.7	6.6
-1	3	2	35.2	1.5
1	5	2	195.6	5.5
-1	5	2	1431.9	12.5
1	7	2	199.8	8.3
-1	7	2	2567.3	10.3
1	9	2	4093.8	14.6
-1	9	2	2.8	1.3
1	11	2	9018.3	117.5
-1	11	2	104.2	2.9
1	13	2	407.0	5.6
-1	13	2	1222.0	9.2
1	15	2	629.4	20.0
-1	15	2	672.3	13.6
1	17	2	1.6	2.8
-1	17	2	22.6	2.8
1	19	2	187.5	5.0
-1	19	2	18.1	3.4
1	21	2	93.5	10.0
-1	21	2	507.5	8.2
1	23	2	370.5	7.7
-1	23	2	178.9	6.0
2	0	2	12041.1	30.3
-2	0	2	20816.1	35.2
2	2	2	491.4	4.6
-2	2	2	876.4	8.1
2	4	2	1864.9	19.7
-2	4	2	3102.7	21.5
2	6	2	32.3	1.8
-2	6	2	76.6	3.8
2	8	2	81.3	2.7
-2	8	2	5094.9	28.6
2	10	2	765.1	7.0
-2	10	2	1860.8	22.7
2	12	2	270.2	4.7
-2	12	2	16518.5	31.9

## fluoro-tremolite 1082\_751\_361.cif

2	14	2	109.5	4.1
-2	14	2	34.3	2.5
2	16	2	374.8	13.4
-2	16	2	1446.4	21.3
2	18	2	126.8	8.9
-2	18	2	271.9	5.6
2	20	2	1493.7	14.6
-2	20	2	1319.1	12.4
2	22	2	1187.1	14.4
-2	22	2	1910.9	15.9
-2	24	2	1970.9	33.8
3	1	2	473.6	11.1
-3	1	2	6298.8	51.5
3	3	2	578.2	7.1
-3	3	2	1749.7	7.9
3	5	2	278.4	4.0
-3	5	2	2114.6	16.5
3	7	2	1246.3	12.6
-3	7	2	1002.2	7.9
3	9	2	0.1	1.6
-3	9	2	1085.3	7.6
3	11	2	12.1	2.3
-3	11	2	5276.3	77.8
3	13	2	1458.5	29.1
-3	13	2	13.0	2.2
3	15	2	563.9	10.3
-3	15	2	1.5	2.3
3	17	2	15.1	7.8
-3	17	2	9.5	3.3
3	19	2	42.7	3.3
-3	19	2	316.5	6.2
3	21	2	528.3	12.2
-3	21	2	49.9	4.3
3	23	2	631.2	10.1
-3	23	2	510.8	8.9
4	0	2	8909.4	30.6
-4	0	2	9463.1	27.8
4	2	2	869.2	7.0
-4	2	2	556.0	8.0
4	4	2	3601.3	29.5
-4	4	2	2367.0	23.1
4	6	2	29.2	2.1
-4	6	2	8.5	1.8
4	8	2	307.3	13.2
-4	8	2	2960.0	12.5
4	10	2	406.0	8.7
-4	10	2	387.3	5.7
4	12	2	4919.4	45.3
-4	12	2	24.3	3.0
4	14	2	14.9	2.7
-4	14	2	257.8	4.9
4	16	2	136.0	4.5
-4	16	2	140.2	6.9
4	18	2	513.0	8.1
-4	18	2	395.3	6.7
4	20	2	28.8	3.5
-4	20	2	138.9	4.8
4	22	2	660.0	11.6
-4	22	2	401.7	7.9
5	1	2	12608.0	147.1
-5	1	2	3403.2	21.6
5	3	2	3585.2	15.1
-5	3	2	135.6	2.8
5	5	2	1329.2	10.8
-5	5	2	280.3	4.0
5	7	2	249.5	4.5
-5	7	2	9.4	3.7
5	9	2	1930.5	22.9
-5	9	2	3244.3	15.0
5	11	2	10882.0	105.5
-5	11	2	13392.0	271.0
5	13	2	889.3	19.4
-5	13	2	1173.6	9.9
5	15	2	321.0	6.3
-5	15	2	446.8	12.9
5	17	2	28.6	3.4
-5	17	2	21.1	3.1
5	19	2	1009.4	16.3
-5	19	2	47.0	3.7
5	21	2	35.2	4.0
-5	21	2	134.4	5.2
-5	23	2	1118.6	13.2
6	0	2	2477.8	19.1
-6	0	2	17227.3	43.4
6	2	2	33.7	2.4
-6	2	2	60.2	2.5
6	4	2	355.9	5.5
-6	4	2	3086.6	13.3
6	6	2	331.6	5.4
-6	6	2	4.5	2.3
6	8	2	3.3	2.1
-6	8	2	1101.1	8.8
6	10	2	618.3	7.8
-6	10	2	1496.4	10.6
6	12	2	163.8	4.6
-6	12	2	1779.1	14.1

## fluoro-tremolite 1082\_751\_361.cif

6	14	2	165.2	7.6
-6	14	2	106.1	3.7
6	16	2	134.5	6.1
-6	16	2	888.3	9.8
6	18	2	50.1	4.0
-6	18	2	158.1	4.9
6	20	2	46.6	4.1
-6	20	2	2794.4	33.7
-6	22	2	1800.6	16.3
7	1	2	270.0	5.1
-7	1	2	570.2	6.2
7	3	2	1930.3	13.0
-7	3	2	1481.0	21.0
7	5	2	367.0	6.0
-7	5	2	165.9	3.7
7	7	2	644.9	8.0
-7	7	2	998.5	8.7
7	9	2	4.8	5.1
-7	9	2	158.2	4.0
7	11	2	419.5	12.4
-7	11	2	14.6	2.4
7	13	2	119.8	4.4
-7	13	2	980.5	9.8
7	15	2	311.9	6.8
-7	15	2	865.1	19.1
7	17	2	48.0	3.9
-7	17	2	0.4	3.8
7	19	2	260.0	6.9
-7	19	2	26.6	3.5
-7	21	2	917.8	15.0
8	0	2	6436.0	34.9
-8	0	2	732.9	11.0
8	2	2	74.7	3.5
-8	2	2	170.9	4.0
8	4	2	1202.4	11.1
-8	4	2	2644.9	17.4
8	6	2	115.1	4.2
-8	6	2	74.3	3.1
8	8	2	242.3	5.6
-8	8	2	6.0	2.3
8	10	2	431.4	7.5
-8	10	2	197.5	4.7
8	12	2	201.9	5.6
-8	12	2	380.8	6.5
8	14	2	49.0	3.8
-8	14	2	175.7	4.9
8	16	2	221.8	6.3
-8	16	2	157.4	5.0
-8	18	2	681.8	9.9
-8	20	2	11.7	4.2
9	1	2	162.6	4.9
-9	1	2	2344.0	14.2
9	3	2	2.0	2.9
-9	3	2	2283.8	22.3
9	5	2	344.7	6.7
-9	5	2	1259.7	10.8
9	7	2	68.4	5.5
-9	7	2	79.3	3.5
9	9	2	360.6	9.7
-9	9	2	1612.1	12.7
9	11	2	1313.5	13.3
-9	11	2	2483.8	16.3
9	13	2	5.8	3.8
-9	13	2	12.6	3.1
9	15	2	26.2	4.2
-9	15	2	191.8	6.4
-9	17	2	7.6	3.3
-9	19	2	834.7	11.6
10	0	2	864.3	15.3
-10	0	2	2386.3	21.7
10	2	2	78.1	11.1
-10	2	2	386.8	6.5
10	4	2	1784.1	15.0
-10	4	2	393.2	6.6
10	6	2	18.9	3.7
-10	6	2	412.8	6.8
10	8	2	382.1	7.7
-10	8	2	5.3	2.9
10	10	2	19.5	3.7
-10	10	2	88.4	7.9
10	12	2	824.7	11.5
-10	12	2	305.8	21.0
-10	14	2	7.5	3.6
-10	16	2	67.3	4.4
11	1	2	95.3	4.8
-11	1	2	458.7	7.6
11	3	2	345.3	7.6
-11	3	2	940.1	10.5
11	5	2	36.6	4.4
-11	5	2	92.3	4.8
11	7	2	690.7	10.5
-11	7	2	454.5	9.5
11	9	2	213.1	6.5
-11	9	2	59.5	3.7
-11	11	2	198.8	14.2
-11	13	2	270.6	6.7

## fluoro-tremolite 1082\_751\_361.cif

-11	15	2	162.7	8.9
-12	0	2	7579.7	43.1
-12	2	2	516.7	8.5
-12	4	2	421.0	7.9
-12	6	2	35.7	3.7
-12	8	2	78.1	4.4
-12	10	2	65.8	4.5
-12	12	2	729.6	10.9
-13	1	2	2193.5	17.8
-13	3	2	97.8	4.9
-13	5	2	130.8	5.4
-13	7	2	8.9	4.1
0	0	3	762.1	8.6
0	2	3	4749.4	15.0
0	4	3	10.2	1.6
0	6	3	1078.7	41.3
0	8	3	3.4	2.2
0	10	3	1064.6	8.6
0	12	3	178.5	4.0
0	14	3	192.5	4.5
0	16	3	811.3	15.5
0	18	3	167.2	4.9
0	20	3	227.1	6.4
0	22	3	15.4	3.8
1	1	3	465.2	5.5
-1	1	3	206.7	6.1
1	3	3	9.9	2.3
-1	3	3	5256.2	140.4
1	5	3	762.3	15.3
-1	5	3	16069.8	586.6
1	7	3	496.8	9.7
-1	7	3	3459.1	15.8
1	9	3	1198.1	15.3
-1	9	3	1209.4	12.1
1	11	3	4.3	2.2
-1	11	3	899.9	9.6
1	13	3	200.0	4.6
-1	13	3	-0.3	1.8
1	15	3	1.8	4.2
-1	15	3	492.0	8.3
1	17	3	304.3	6.2
-1	17	3	4974.1	25.7
1	19	3	-1.6	3.2
-1	19	3	355.1	7.1
1	21	3	54.2	4.0
-1	21	3	422.2	7.9
-1	23	3	262.6	6.9
2	0	3	276.5	5.8
-2	0	3	148.7	3.9
2	2	3	1880.0	28.6
-2	2	3	36.4	2.5
2	4	3	8.4	1.7
-2	4	3	3.4	1.4
2	6	3	6553.5	20.3
-2	6	3	17493.4	45.6
2	8	3	132.1	3.5
-2	8	3	125.7	3.1
2	10	3	2818.2	14.6
-2	10	3	4.0	6.6
2	12	3	166.9	4.2
-2	12	3	204.1	4.2
2	14	3	2492.3	15.4
-2	14	3	2522.4	14.6
2	16	3	1640.2	13.2
-2	16	3	2650.8	16.0
2	18	3	88.8	9.4
-2	18	3	3767.4	31.2
2	20	3	8.2	3.6
-2	20	3	12.2	3.4
2	22	3	138.7	5.4
-2	22	3	278.0	6.8
3	1	3	4.4	2.2
-3	1	3	698.8	6.0
3	3	3	25.6	2.1
-3	3	3	391.0	9.4
3	5	3	591.1	6.6
-3	5	3	688.7	6.1
3	7	3	434.9	9.7
-3	7	3	846.8	7.1
3	9	3	841.5	8.3
-3	9	3	2213.4	13.9
3	11	3	101.5	5.4
-3	11	3	6.2	2.0
3	13	3	22.9	2.8
-3	13	3	1088.7	10.6
3	15	3	3.6	2.6
-3	15	3	355.1	6.2
3	17	3	145.4	5.4
-3	17	3	1.2	3.2
3	19	3	27.1	3.5
-3	19	3	32.3	5.2
3	21	3	37.9	4.1
-3	21	3	61.4	4.1
-3	23	3	279.5	14.9
4	0	3	11.9	2.8
-4	0	3	87.8	3.7

## fluoro-tremolite 1082\_751\_361.cif

4	2	3	1815.1	11.4
-4	2	3	15.1	1.6
4	4	3	194.1	4.7
-4	4	3	5.7	1.6
4	6	3	2414.7	13.7
-4	6	3	596.2	6.1
4	8	3	9.4	2.2
-4	8	3	2.9	2.0
4	10	3	335.0	5.8
-4	10	3	836.1	7.8
4	12	3	280.8	9.1
-4	12	3	417.1	7.6
4	14	3	40.7	3.2
-4	14	3	345.1	5.9
4	16	3	277.2	8.9
-4	16	3	1146.8	26.1
4	18	3	2415.4	46.4
-4	18	3	871.2	24.2
4	20	3	215.3	11.8
-4	20	3	197.4	5.7
-4	22	3	29.9	3.6
5	1	3	1.6	2.2
-5	1	3	64.3	2.4
5	3	3	2251.7	13.5
-5	3	3	2119.9	14.3
5	5	3	3401.3	17.0
-5	5	3	6004.2	19.0
5	7	3	120.2	11.0
-5	7	3	289.4	5.7
5	9	3	574.3	7.7
-5	9	3	24.8	3.3
5	11	3	157.2	4.6
-5	11	3	108.2	3.5
5	13	3	61.3	3.6
-5	13	3	364.4	5.9
5	15	3	335.7	12.5
-5	15	3	871.6	20.3
5	17	3	673.7	9.9
-5	17	3	4080.9	32.1
5	19	3	4.3	9.4
-5	19	3	607.0	10.7
-5	21	3	1087.8	12.6
6	0	3	477.3	9.6
-6	0	3	393.2	7.5
6	2	3	24.8	2.5
-6	2	3	1095.8	16.2
6	4	3	5.4	3.4
-6	4	3	8.7	1.9
6	6	3	9309.5	29.6
-6	6	3	51.8	2.5
6	8	3	156.9	4.7
-6	8	3	9.3	2.2
6	10	3	28.9	3.3
-6	10	3	10.8	2.1
6	12	3	4.6	3.4
-6	12	3	166.1	4.3
6	14	3	1504.0	17.6
-6	14	3	8.7	2.3
6	16	3	1245.6	24.7
-6	16	3	685.2	9.1
6	18	3	2759.0	20.3
-6	18	3	1193.1	12.9
-6	20	3	334.0	7.4
7	1	3	104.1	4.9
-7	1	3	91.0	3.1
7	3	3	32.9	3.9
-7	3	3	3.2	2.3
7	5	3	398.5	6.9
-7	5	3	246.1	4.7
7	7	3	75.9	7.4
-7	7	3	2607.7	14.5
7	9	3	740.1	9.5
-7	9	3	660.1	7.8
7	11	3	100.3	7.1
-7	11	3	325.3	14.5
7	13	3	176.9	6.0
-7	13	3	773.2	9.1
7	15	3	88.0	4.7
-7	15	3	118.2	5.7
-7	17	3	950.6	11.3
-7	19	3	621.1	9.7
8	0	3	2.8	3.9
-8	0	3	169.7	6.0
8	2	3	127.8	4.6
-8	2	3	29.4	14.8
8	4	3	52.5	3.6
-8	4	3	234.3	12.1
8	6	3	1077.1	11.7
-8	6	3	7962.9	26.2
8	8	3	111.6	4.8
-8	8	3	428.1	6.6
8	10	3	24.8	3.3
-8	10	3	0.9	2.8
8	12	3	313.4	16.0
-8	12	3	92.3	4.0
8	14	3	0.1	3.4

## fluoro-tremolite 1082\_751\_361.cif

-8	14	3	1803.7	14.7
-8	16	3	947.7	11.2
-8	18	3	2053.5	17.2
9	1	3	0.3	3.8
-9	1	3	27.9	2.9
9	3	3	571.8	9.0
-9	3	3	1135.6	10.5
9	5	3	4566.6	24.5
-9	5	3	6179.9	24.2
9	7	3	812.9	10.9
-9	7	3	771.3	9.1
9	9	3	33.4	4.0
-9	9	3	68.1	3.5
9	11	3	-1.0	4.1
-9	11	3	308.3	6.4
-9	13	3	2.3	3.0
-9	15	3	179.0	5.5
-9	17	3	2438.4	19.2
10	0	3	206.0	8.6
-10	0	3	223.7	7.3
10	2	3	22.0	3.7
-10	2	3	773.6	9.3
10	4	3	92.2	4.8
-10	4	3	25.2	3.0
10	6	3	150.1	14.2
-10	6	3	81.9	4.0
10	8	3	224.0	16.8
-10	8	3	5.1	3.6
-10	10	3	7.4	3.4
-10	12	3	68.9	4.1
-10	14	3	39.3	4.3
-10	16	3	385.8	10.9
-11	1	3	222.4	8.4
-11	3	3	141.3	4.8
-11	5	3	1644.2	14.3
-11	7	3	3.0	3.9
-11	9	3	164.5	5.3
-11	11	3	26.6	3.4
-11	13	3	60.6	4.7
-12	0	3	7.1	5.4
-12	2	3	389.4	15.2
-12	4	3	124.8	5.0
-12	6	3	5133.2	26.3
-12	8	3	13.2	3.4
-12	10	3	735.2	10.7
-13	1	3	24.7	3.6
-13	3	3	9.0	4.8
-13	5	3	154.7	7.4
-13	7	3	158.4	18.3
0	0	4	8966.9	33.9
0	2	4	164.1	3.7
0	4	4	719.8	7.3
0	6	4	70.2	3.0
0	8	4	814.3	8.2
0	10	4	936.6	9.2
0	12	4	4671.0	20.7
0	14	4	9.8	4.2
0	16	4	451.2	12.5
0	18	4	175.2	5.3
0	20	4	296.1	7.1
1	1	4	19.0	2.1
-1	1	4	8074.0	41.4
1	3	4	623.5	6.9
-1	3	4	2566.6	20.3
1	5	4	14.5	2.3
-1	5	4	916.5	8.2
1	7	4	840.1	8.4
-1	7	4	495.0	7.3
1	9	4	13.4	3.3
-1	9	4	1281.9	10.2
1	11	4	356.1	6.2
-1	11	4	6654.6	47.0
1	13	4	356.1	7.1
-1	13	4	230.5	6.1
1	15	4	316.0	6.4
-1	15	4	137.0	4.5
1	17	4	-0.4	3.7
-1	17	4	147.2	4.9
1	19	4	58.4	4.2
-1	19	4	791.1	10.6
-1	21	4	16.9	7.2
2	0	4	13830.6	44.9
-2	0	4	1264.1	12.6
2	2	4	391.9	5.7
-2	2	4	245.2	5.3
2	4	4	35.9	3.6
-2	4	4	646.7	11.2
2	6	4	17.9	2.2
-2	6	4	7.1	7.3
2	8	4	162.0	10.8
-2	8	4	7.3	2.3
2	10	4	344.6	6.1
-2	10	4	152.7	4.0
2	12	4	1512.2	16.4
-2	12	4	1784.4	12.7
2	14	4	6.9	3.3

## fluoro-tremolite 1082\_751\_361.cif

-2	14	4	261.2	5.5
2	16	4	7.4	3.8
-2	16	4	316.1	8.9
2	18	4	284.2	6.8
-2	18	4	495.7	7.5
2	20	4	473.3	8.9
-2	20	4	9.4	3.5
3	1	4	2871.8	16.3
-3	1	4	1533.8	10.4
3	3	4	35.0	2.6
-3	3	4	2044.9	11.4
3	5	4	22.0	3.8
-3	5	4	4.7	2.9
3	7	4	173.5	4.5
-3	7	4	376.7	5.5
3	9	4	2008.7	14.0
-3	9	4	8.6	3.0
3	11	4	9018.5	47.2
-3	11	4	36.8	2.8
3	13	4	977.2	10.8
-3	13	4	761.3	18.2
3	15	4	461.1	14.7
-3	15	4	340.5	7.1
3	17	4	18.5	3.4
-3	17	4	5.7	3.1
3	19	4	233.6	6.7
-3	19	4	67.4	4.1
-3	21	4	667.2	25.7
4	0	4	58.9	4.5
-4	0	4	12972.1	41.1
4	2	4	12.6	3.3
-4	2	4	402.9	5.6
4	4	4	147.3	4.3
-4	4	4	1516.7	10.2
4	6	4	138.7	4.4
-4	6	4	9.5	2.2
4	8	4	122.8	4.3
-4	8	4	207.3	4.4
4	10	4	243.6	23.0
-4	10	4	494.0	6.7
4	12	4	1120.7	11.8
-4	12	4	832.3	18.0
4	14	4	395.2	7.7
-4	14	4	14.2	2.8
4	16	4	125.9	6.3
-4	16	4	270.7	6.0
4	18	4	35.1	4.0
-4	18	4	154.4	5.2
-4	20	4	1971.1	22.0
5	1	4	155.0	4.5
-5	1	4	32.2	2.5
5	3	4	194.3	5.0
-5	3	4	-1.7	2.6
5	5	4	14.5	3.5
-5	5	4	191.0	5.4
5	7	4	1414.8	23.9
-5	7	4	1.6	2.1
5	9	4	131.6	4.7
-5	9	4	1559.4	13.5
5	11	4	163.7	6.6
-5	11	4	2525.7	42.7
5	13	4	1060.2	12.0
-5	13	4	15.4	4.7
5	15	4	562.5	25.7
-5	15	4	85.3	3.9
-5	17	4	68.9	7.1
-5	19	4	108.3	4.9
6	0	4	1840.8	20.2
-6	0	4	134.8	5.6
6	2	4	178.9	5.0
-6	2	4	422.7	6.1
6	4	4	17.3	8.0
-6	4	4	3851.0	17.5
6	6	4	31.6	4.7
-6	6	4	72.4	3.1
6	8	4	1801.2	14.9
-6	8	4	1227.0	21.1
6	10	4	268.2	11.6
-6	10	4	58.8	3.3
6	12	4	1455.7	14.3
-6	12	4	172.4	4.7
6	14	4	3.6	3.6
-6	14	4	90.4	8.8
-6	16	4	64.5	3.9
-6	18	4	236.9	6.2
7	1	4	349.7	7.0
-7	1	4	3876.2	18.3
7	3	4	106.5	4.5
-7	3	4	885.2	9.1
7	5	4	521.6	10.3
-7	5	4	432.5	6.4
7	7	4	3.9	3.9
-7	7	4	915.0	9.4
7	9	4	293.7	7.0
-7	9	4	514.8	9.5
7	11	4	661.5	13.9

## fluoro-tremolite 1082\_751\_361.cif

-7	11	4	3438.7	18.9
7	13	4	12.5	3.6
-7	13	4	10.1	3.5
-7	15	4	-1.3	3.2
-7	17	4	111.2	4.9
-7	19	4	193.8	6.1
8	0	4	127.3	7.4
-8	0	4	11429.6	46.3
8	2	4	178.9	5.8
-8	2	4	164.0	4.5
8	4	4	460.2	8.5
-8	4	4	59.7	12.6
8	6	4	13.5	3.6
-8	6	4	29.0	2.8
8	8	4	893.2	11.8
-8	8	4	2749.2	23.8
8	10	4	4.8	3.9
-8	10	4	874.4	10.0
-8	12	4	6474.8	27.2
-8	14	4	-0.9	3.7
-8	16	4	1322.0	13.7
-8	18	4	123.5	5.4
9	1	4	162.5	5.9
-9	1	4	58.5	3.5
9	3	4	10.5	4.2
-9	3	4	624.4	11.1
9	5	4	153.8	6.0
-9	5	4	29.0	3.0
-9	7	4	436.9	7.3
-9	9	4	10.4	4.3
-9	11	4	817.0	14.0
-9	13	4	41.8	3.8
-9	15	4	285.4	7.0
-10	0	4	387.1	10.2
-10	2	4	28.4	13.0
-10	4	4	16.4	7.1
-10	6	4	117.8	4.5
-10	8	4	450.5	13.2
-10	10	4	256.5	14.4
-10	12	4	978.9	12.0
-10	14	4	359.0	8.0
-11	1	4	328.8	9.3
-11	3	4	83.1	4.2
-11	5	4	53.7	3.9
-11	7	4	57.7	3.9
-11	9	4	1676.4	15.5
-11	11	4	2990.7	20.9
-12	0	4	1137.4	18.2
-12	2	4	85.7	4.7
-12	4	4	119.4	5.1
-12	6	4	162.5	5.7
-12	8	4	12.5	4.0
-13	1	4	360.9	8.1
-13	3	4	233.3	21.3
0	0	5	101.6	5.2
0	2	5	938.4	9.4
0	4	5	6.6	4.1
0	6	5	2865.7	34.2
0	8	5	69.2	3.5
0	10	5	671.1	8.9
0	12	5	94.9	5.0
0	14	5	3832.1	36.2
0	16	5	1237.3	13.1
0	18	5	602.7	10.0
1	1	5	26.1	5.5
-1	1	5	102.2	3.6
1	3	5	35.1	3.1
-1	3	5	16.3	3.4
1	5	5	588.2	14.0
-1	5	5	318.3	5.9
1	7	5	24.7	4.9
-1	7	5	393.6	6.5
1	9	5	248.1	5.8
-1	9	5	223.2	5.4
1	11	5	267.7	6.2
-1	11	5	39.4	3.5
1	13	5	155.3	5.7
-1	13	5	400.0	7.3
1	15	5	68.3	4.4
-1	15	5	13.2	3.1
1	17	5	20.0	3.6
-1	17	5	9.1	4.4
2	0	5	29.1	4.1
-2	0	5	206.5	6.5
2	2	5	1275.7	11.5
-2	2	5	1834.1	12.5
2	4	5	30.2	3.3
-2	4	5	140.7	4.2
2	6	5	38.1	3.4
-2	6	5	1022.5	10.0
2	8	5	32.0	3.3
-2	8	5	16.8	2.8
2	10	5	191.4	5.5
-2	10	5	154.6	5.4
2	12	5	349.3	7.2
-2	12	5	66.8	3.6

## fluoro-tremolite 1082\_751\_361.cif

2	14	5	126.1	7.1
-2	14	5	293.5	6.4
2	16	5	249.4	13.0
-2	16	5	252.3	8.0
-2	18	5	2457.1	19.1
3	1	5	1.9	3.1
-3	1	5	61.1	2.9
3	3	5	1624.3	15.0
-3	3	5	1050.8	9.7
3	5	5	4363.3	69.4
-3	5	5	3440.1	17.4
3	7	5	484.5	7.9
-3	7	5	64.7	3.3
3	9	5	192.5	5.6
-3	9	5	4.9	3.3
3	11	5	2.0	3.5
-3	11	5	142.3	4.6
3	13	5	99.8	4.8
-3	13	5	142.5	4.8
3	15	5	816.7	11.5
-3	15	5	602.2	9.1
-3	17	5	2302.0	17.8
4	0	5	297.3	8.9
-4	0	5	235.7	6.7
4	2	5	50.2	36.8
-4	2	5	4.7	4.3
4	4	5	9.0	3.6
-4	4	5	10.8	2.6
4	6	5	7404.6	78.9
-4	6	5	11734.7	64.6
4	8	5	8.0	3.9
-4	8	5	226.5	9.0
4	10	5	222.5	6.1
-4	10	5	200.3	5.1
4	12	5	0.2	3.4
-4	12	5	97.4	4.1
4	14	5	268.0	7.2
-4	14	5	486.3	12.1
-4	16	5	1135.1	12.6
-4	18	5	1349.3	14.4
5	1	5	74.7	4.3
-5	1	5	305.8	8.3
5	3	5	331.4	7.0
-5	3	5	13.3	2.3
5	5	5	147.4	5.2
-5	5	5	541.6	16.5
5	7	5	229.3	6.2
-5	7	5	143.0	4.3
5	9	5	829.0	27.3
-5	9	5	823.0	13.5
5	11	5	29.1	5.5
-5	11	5	57.5	3.4
-5	13	5	521.9	10.7
-5	15	5	115.9	7.9
-5	17	5	55.6	4.3
6	0	5	15.9	6.4
-6	0	5	79.1	4.9
6	2	5	67.6	4.3
-6	2	5	181.9	4.8
6	4	5	30.6	4.3
-6	4	5	13.0	3.3
6	6	5	21.0	4.8
-6	6	5	986.7	17.2
6	8	5	7.6	3.9
-6	8	5	12.4	3.9
6	10	5	9.5	3.8
-6	10	5	16.0	8.6
-6	12	5	196.2	6.7
-6	14	5	621.1	14.1
-6	16	5	885.4	11.4
7	1	5	4.8	4.4
-7	1	5	19.5	3.1
7	3	5	518.9	9.4
-7	3	5	1551.2	13.0
7	5	5	1976.0	31.9
-7	5	5	7710.7	86.0
-7	7	5	1577.6	13.3
-7	9	5	328.9	6.5
-7	11	5	179.8	8.0
-7	13	5	7.5	3.0
-7	15	5	196.6	8.8
-8	0	5	74.1	5.5
-8	2	5	78.3	6.7
-8	4	5	13.2	3.5
-8	6	5	111.1	4.5
-8	8	5	67.0	4.0
-8	10	5	48.8	4.2
-8	12	5	120.1	4.9
-8	14	5	283.0	6.9
-9	1	5	80.8	5.5
-9	3	5	143.5	5.0
-9	5	5	387.1	13.8
-9	7	5	2114.6	16.5
-9	9	5	1186.3	23.0
-9	11	5	33.7	4.5
-9	13	5	189.1	6.0

## fluoro-tremolite 1082\_751\_361.cif

-10	0	5	72.4	5.8
-10	2	5	35.2	3.6
-10	4	5	112.9	5.7
-10	6	5	1950.2	16.4
-10	8	5	122.6	11.7
-10	10	5	89.6	4.5
-10	12	5	138.5	5.5
-11	1	5	41.1	4.7
-11	3	5	634.8	10.0
-11	5	5	1520.4	15.2
-11	7	5	17.0	5.3
-11	9	5	11.5	5.7
-12	0	5	415.2	12.3
-12	2	5	815.7	11.7
-12	4	5	180.5	6.3
0	0	6	1163.7	16.9
0	2	6	216.4	5.7
0	4	6	242.6	6.1
0	6	6	2.3	3.0
0	8	6	518.0	8.7
0	10	6	141.3	5.4
0	12	6	806.0	11.3
1	1	6	1660.2	14.4
-1	1	6	216.8	5.5
1	3	6	378.2	7.3
-1	3	6	536.3	8.2
1	5	6	502.6	12.2
-1	5	6	28.7	3.5
1	7	6	117.7	4.9
-1	7	6	550.3	8.7
1	9	6	228.1	6.4
-1	9	6	33.7	3.8
1	11	6	1474.0	15.0
-1	11	6	1.6	3.7
1	13	6	8.9	4.5
-1	13	6	645.8	13.3
2	0	6	799.1	14.8
-2	0	6	7540.9	40.0
2	2	6	31.9	3.6
-2	2	6	113.3	4.4
2	4	6	256.4	9.5
-2	4	6	5.0	3.0
2	6	6	55.4	4.2
-2	6	6	55.7	3.8
2	8	6	55.0	4.4
-2	8	6	214.4	39.7
2	10	6	94.0	5.1
-2	10	6	261.7	6.6
-2	12	6	924.0	11.6
-2	14	6	52.4	4.1
3	1	6	330.2	11.7
-3	1	6	2830.4	31.9
3	3	6	215.7	6.3
-3	3	6	284.8	6.0
3	5	6	96.9	7.1
-3	5	6	11.1	10.9
3	7	6	173.6	5.9
-3	7	6	76.6	4.0
3	9	6	194.8	6.2
-3	9	6	2421.3	17.4
-3	11	6	8310.3	32.5
-3	13	6	1014.2	12.2
4	0	6	7557.7	46.6
-4	0	6	1134.1	15.9
4	2	6	175.6	6.2
-4	2	6	111.4	4.2
4	4	6	484.8	9.2
-4	4	6	46.0	10.2
4	6	6	16.1	4.1
-4	6	6	3.9	3.0
-4	8	6	42.8	3.7
-4	10	6	209.6	5.9
-4	12	6	37.7	5.4
-4	14	6	78.5	6.7
5	1	6	317.7	12.0
-5	1	6	3.4	5.3
-5	3	6	292.9	14.6
-5	5	6	47.5	3.4
-5	7	6	973.2	11.0
-5	9	6	56.3	3.9
-5	11	6	25.7	3.8
-5	13	6	302.1	12.1
-6	0	6	1803.7	20.8
-6	2	6	86.0	6.3
-6	4	6	9.7	5.9
-6	6	6	1.7	2.8
-6	8	6	1798.7	15.2
-6	10	6	446.0	12.3
-6	12	6	1204.6	13.3
-7	1	6	229.3	8.1
-7	3	6	118.2	5.1
-7	5	6	484.7	8.2
-7	7	6	103.1	4.6
-7	9	6	286.9	6.8
-7	11	6	569.9	9.4
-8	0	6	187.9	6.7

fluoro-tremolite 1082\_751\_361.cif

```

-8 2 6 214.6 6.0
-8 4 6 1067.3 12.2
-8 6 6 49.7 3.9
-8 8 6 1179.1 13.1
-8 10 6 6.7 8.2
-9 1 6 16.3 3.9
-9 3 6 66.9 4.6
-9 5 6 -0.4 3.6
-9 7 6 21.7 4.1
-9 9 6 738.3 13.6
-10 0 6 8331.0 50.4
-10 2 6 361.7 8.2
-10 4 6 289.8 7.3
-10 6 6 69.3 4.7
0 0 7 -0.8 4.4
0 2 7 768.5 43.2
0 4 7 54.0 4.4
1 1 7 2.6 3.6
-1 1 7 4.1 9.8
-1 3 7 -0.1 3.6
-1 5 7 606.9 9.9
-1 7 7 32.3 4.4
-2 0 7 41.7 5.5
-2 2 7 433.8 8.3
-2 4 7 -0.1 3.5
-2 6 7 4801.6 75.7
-2 8 7 41.7 5.6
-3 1 7 90.1 4.4
-3 3 7 118.4 10.0
-3 5 7 564.1 26.9
-3 7 7 9.2 4.2
-4 0 7 136.6 7.1
-4 2 7 695.1 10.1
-4 4 7 17.4 3.3
-4 6 7 1370.4 14.5
-4 8 7 0.7 3.2
-5 1 7 13.8 2.8
-5 3 7 304.0 7.2
-5 5 7 680.1 10.4
-5 7 7 5.0 3.2
-6 0 7 130.3 7.1
-6 2 7 1.9 3.2
-6 4 7 77.8 4.5
-6 6 7 2490.0 32.9
-7 1 7 37.6 3.7
-7 3 7 14.9 4.5

```

#====END

data\_751\_EJE

```

_publ_contact_author
;
Roberta Oberti
;
_publ_contact_author_email
;
oberti@crystal.unipv.it
;

loop_
_publ_author_name
_publ_author_address
'Oberti R.'
'CNR-IGG, S.S. Pavia, Pavia, Italy'
'Camara F.'
'Dip.to di Scienze della Terra, Università di Milano, Milan, Italy'
'Bellatreccia F.'
'Dip.to di Scienze, Università Roma Tre, Rome, Italy'
'Radica F.'
'Dip.to di Scienze, Università Roma Tre, Rome, Italy'
'Gianfagna A.'
'Dip.to di Scienze della Terra, Università di Roma La Sapienza, Rome, Italy'
'Boiocchi M.'
'Centro Grandi Strumenti, Università di Pavia, Pavia, Italy'

_publ_section_title
;
Fluoro-tremolite from the Limecrest-Southdown quarry, Sparta, NJ, USA:
crystal structure and crystal chemistry of a newly approved end-members
of the amphibole supergroup and its solid solution with tremolite
;

_audit_creation_method      'manually entered'
_chemical_name_systematic   ?
_chemical_name_mineral      ?
_chemical_compound_source   ?
_chemical_name_common        ;
synthetic fluoro-tremolite
;
_chemical_melting_point     ?
_chemical_formula_moietry   ?
_chemical_formula_sum        ?
_A10.13 Ca1.71 F1.98 Fe0.06 Mg5.28 O22.02 Si8'
_chemical_formula_weight     818.86

```

```

loop_
  _atom_type_symbol
  _atom_type_description
  _atom_type_scat_dispersion_real
  _atom_type_scat_dispersion_imag
  _atom_type_scat_source
  'O'  'O'  0.0106  0.0060
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'O2-'  'O2-'  0.0106  0.0060
  'Hovesteydt, 1982'
  'O-'  'O-'  0.0106  0.0060
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'F-'  'F-'  0.0140  0.0100
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'Si'  'Si'  0.0817  0.0704
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'Si4+'  'Si4+'  0.0817  0.0710
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'Al3+'  'Al3+'  0.0645  0.0520
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'Mg2+'  'Mg2+'  0.0490  0.0360
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'Ca2+'  'Ca2+'  0.2260  0.3060
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
  'Fe2+'  'Fe2+'  0.3460  0.8450
  'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

  _space_group_crystal_system      monoclinic
  _space_group_IT_number          12
  _space_group_name_H-M_alt       'C 2/m'
  _space_group_name_Hall          '-C 2y'

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

  _cell_length_a                  9.784(2)
  _cell_length_b                  18.015(4)
  _cell_length_c                  5.272(2)
  _cell_angle_alpha                90
  _cell_angle_beta                 104.522(19)
  _cell_angle_gamma                90
  _cell_volume                     899.6(4)
  _cell_formula_units_Z            2
  _cell_measurement_temperature    298(2)
  _cell_measurement_reflns_used   60
  _cell_measurement_theta_min     2
  _cell_measurement_theta_max     30

  _exptl_crystal_description      'prism'
  _exptl_crystal_colour           'colourless'
  _exptl_crystal_density_meas     ?
  _exptl_crystal_density_method   ?
  _exptl_crystal_density_diffnn  3.023
  _exptl_crystal_F_000             814.00
  _exptl_crystal_size_max          0.460
  _exptl_crystal_size_mid          0.260
  _exptl_crystal_size_min          0.230
  _exptl_absorpt_coefficient_mu   1.472
  _exptl_absorpt_correction_type   psi-scan
  _exptl_absorpt_correction_T_min  0.717
  _exptl_absorpt_correction_T_max  0.815
  _exptl_absorpt_process_details   ;
  North A.C.T., Phillips D.C. & Mathews F.S. (1968) Acta. Cryst. A24, 351
  ;
  _exptl_absorpt_special_details   ?

  _diffrn_ambient_temperature     298(2)
  _diffrn_radiation_wavelength    0.7107
  _diffrn_radiation_type          MoK\alpha
  _diffrn_radiation_source         'fine-focus sealed tube'
  _diffrn_radiation_monochromator  graphite
  _diffrn_measurement_device_type  'PHILIPS PW1100'
  _diffrn_measurement_method       'omega-2theta scans'
  _diffrn_standards_number         3
  _diffrn_standards_interval_count 400
  _diffrn_standards_decay_%        0
  _diffrn_reflns_number            2732
  _diffrn_reflns_av_R_equivalents  0.022
  _diffrn_reflns_limit_h_min       -13
  _diffrn_reflns_limit_h_max       13
  _diffrn_reflns_limit_k_min       -25
  _diffrn_reflns_limit_k_max       25
  _diffrn_reflns_limit_l_min       0
  _diffrn_reflns_limit_l_max       7
  _diffrn_reflns_theta_min          2.261
  _diffrn_reflns_theta_max          38.051

```

```

fluoro-tremolite 1082_751_361.cif
_diffrn_measured_fraction_theta_max 1.000
_reflns_number_total 1368
_reflns_number_gt 1007
_reflns_threshold_expression 'I > 3\s(I)'

_computing_data_collection 'local program'
_computing_cell_refinement 'LAT routine of PW1100 diffractometer'
_computing_data_reduction 'local program'
_computing_structure_refinement 'ORFLS (Busing et al., 1962), modified'

_refine_special_details
;
Refinement of F against reflections with F > 3sigma(F).
The threshold expression (_gt) of F > 3sigma(F) corresponds to the cutoff used
to discriminate between observed and unobserved reflections for refinement.
The use of unitary weight produces unusual values for the calculated
weighted wr-factor (similar to R).
;

_refine_ls_structure_factor_coef F
_refine_ls_matrix_type full
_refine_ls_weighting_scheme unit
_refine_ls_extinction_method 'secondary isotropic'
_refine_ls_extinction_coef 0.000030(3)
_refine_ls_extinction_expression 'Zachariasen, 1967'
_refine_ls_number_reflns 1007
_refine_ls_number_parameters 119
_refine_ls_R_factor_all 0.0332
_refine_ls_R_factor_gt 0.0166
_refine_ls_wr_factor_ref 0.0367
_refine_ls_wr_factor_gt 0.0163
_refine_ls_restrained_S_all 1.82

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
O1A 0 0.11235(11) 0.08489(6) 0.2178(2) 0.0061(3) Uani 0.18(9) 1 d . . P . .
O1B 02- 0.11235(11) 0.08489(6) 0.2178(2) 0.0061(3) Uani 0.82(9) 1 d . . P . .
O2A 0 0.11921(11) 0.17018(6) 0.7240(2) 0.0067(3) Uani 0.26(9) 1 d . . P . .
O2B 02- 0.11921(11) 0.17018(6) 0.7240(2) 0.0067(3) Uani 0.74(9) 1 d . . P . .
O3A 0- 0.10271(14) 0.0000 0.7122(3) 0.0080(4) Uani 0.01(3) 2 d S T P . .
O3B F- 0.10271(14) 0.0000 0.7122(3) 0.0080(4) Uani 0.99(3) 2 d S T P . .
O4A 0 0.36560(12) 0.24852(6) 0.7896(2) 0.0100(3) Uani 0.28(10) 1 d . . P . .
O4B 02- 0.36560(12) 0.24852(6) 0.7896(2) 0.0100(3) Uani 0.72(10) 1 d . . P . .
O5A 0 0.34821(11) 0.13531(6) 0.0995(2) 0.0095(3) Uani 0.41(9) 1 d . . P . .
O5B 02- 0.34821(11) 0.13531(6) 0.0995(2) 0.0095(3) Uani 0.59(9) 1 d . . P . .
O6A 0 0.34599(11) 0.11881(6) 0.5882(2) 0.0095(3) Uani 0.36(9) 1 d . . P . .
O6B 02- 0.34599(11) 0.11881(6) 0.5882(2) 0.0095(3) Uani 0.64(9) 1 d . . P . .
O7A 0 0.3417(2) 0.0000 0.2895(3) 0.0106(4) Uani 0.29(7) 2 d S T P . .
O7B 02- 0.3417(2) 0.0000 0.2895(3) 0.0106(4) Uani 0.71(7) 2 d S T P . .
T1A Si 0.28299(4) 0.08376(2) 0.29630(8) 0.0051(2) Uani 0.59(7) 1 d . . P . .
T1B Si4+ 0.28299(4) 0.08376(2) 0.29630(8) 0.0051(2) Uani 0.41(7) 1 d . . P . .
T2A Si 0.29013(4) 0.17084(2) 0.80332(8) 0.0056(2) Uani 0.60(7) 1 d . . P . .
T2B Si4+ 0.29013(4) 0.17084(2) 0.80332(8) 0.0056(2) Uani 0.40(7) 1 d . . P . .
M1A Mg2+ 0.0000 0.08815(4) 0.5000 0.0059(2) Uani 1.00(10) 2 d S T P . .
M1B Al3+ 0.0000 0.08815(4) 0.5000 0.0059(2) Uani 0.00(10) 2 d S T P . .
M2A Mg2+ 0.0000 0.17631(4) 0.0000 0.0055(4) Uani 0.93(10) 2 d S T P . .
M2B Al3+ 0.0000 0.17631(4) 0.0000 0.0055(4) Uani 0.07(10) 2 d S T P . .
M3A Mg2+ 0.0000 0.0000 0.0000 0.0058(6) Uani 1.01(8) 4 d S T P . .
M3B Al3+ 0.0000 0.0000 0.0000 0.0058(6) Uani -0.01(8) 4 d S T P . .
M4A Mg2+ 0.0000 0.27717(4) 0.5000 0.0096(2) Uani 0.207(8) 2 d S T P . .
M4B Ca2+ 0.0000 0.27717(4) 0.5000 0.0096(3) Uani 0.793(8) 2 d S T P . .
AM Ca2+ 0.049(2) 0.5000 0.113(4) 0.032(4) Uiso 0.037(2) 2 d S . P . .
A2 Ca2+ 0.0000 0.4780(13) 0.0000 0.027(5) Uiso 0.026(2) 2 d S . P . .
M42 Fe2+ 0.0000 0.2492(9) 0.5000 0.004(3) Uiso 0.0300(9) 2 d S . P . .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
O1A 0.0058(5) 0.0061(5) 0.0064(5) 0.0001(3) 0.0014(4) -0.0006(4)
O1B 0.0058(5) 0.0061(5) 0.0064(5) 0.0001(3) 0.0014(4) -0.0006(4)
O2A 0.0068(5) 0.0071(5) 0.0060(5) -0.0004(3) 0.0013(4) -0.0001(4)
O2B 0.0068(5) 0.0071(5) 0.0060(5) -0.0004(3) 0.0013(4) -0.0001(4)
O3A 0.0090(6) 0.0072(7) 0.0080(6) 0.0000 0.0022(5) 0.0000
O3B 0.0090(6) 0.0072(7) 0.0080(6) 0.0000 0.0022(5) 0.0000
O4A 0.0122(5) 0.0072(5) 0.0095(5) -0.0031(4) 0.0009(4) -0.0006(4)
O4B 0.0122(5) 0.0072(5) 0.0095(5) -0.0031(4) 0.0009(4) -0.0006(4)
O5A 0.0080(5) 0.0117(5) 0.0084(5) -0.0009(4) 0.0014(4) 0.0034(4)

```

fluoro-tremolite 1082\_751\_361.cif

```

05B 0.0080(5) 0.0117(5) 0.0084(5) -0.0009(4) 0.0014(4) 0.0034(4)
06A 0.0074(5) 0.0118(5) 0.0090(5) 0.0002(4) 0.0013(4) -0.0033(4)
06B 0.0074(5) 0.0118(5) 0.0090(5) 0.0002(4) 0.0013(4) -0.0033(4)
07A 0.0079(7) 0.0074(7) 0.0167(8) 0.0000 0.0034(6) 0.0000
07B 0.0079(7) 0.0074(7) 0.0167(8) 0.0000 0.0034(6) 0.0000
T1A 0.0050(2) 0.0048(2) 0.0055(2) -0.0004(2) 0.0012(2) -0.00051(14)
T1B 0.0050(2) 0.0048(2) 0.0055(2) -0.0004(2) 0.0012(2) -0.00051(14)
T2A 0.0060(2) 0.0056(2) 0.0049(2) -0.0010(2) 0.0009(2) -0.00009(14)
T2B 0.0060(2) 0.0056(2) 0.0049(2) -0.0010(2) 0.0009(2) -0.00009(14)
M1A 0.0068(3) 0.0058(3) 0.0049(3) 0.0000 0.0013(2) 0.0000
M1B 0.0068(3) 0.0058(3) 0.0049(3) 0.0000 0.0013(2) 0.0000
M2A 0.0069(7) 0.0053(7) 0.0047(7) 0.0000 0.0018(3) 0.0000
M2B 0.0069(7) 0.0053(7) 0.0047(7) 0.0000 0.0018(3) 0.0000
M3A 0.0064(10) 0.0054(10) 0.0055(11) 0.0000 0.0012(4) 0.0000
M3B 0.0064(10) 0.0054(10) 0.0055(11) 0.0000 0.0012(4) 0.0000
M4A 0.0113(3) 0.0087(3) 0.0113(3) 0.0000 0.0075(2) 0.0000
M4B 0.0113(3) 0.0087(3) 0.0113(3) 0.0000 0.0075(2) 0.0000

_geom_special_details
;
Geometry data (distances and angles) are reported only for T, M and A
sites flagged by the A suffix.
All esds are estimated using the full covariance matrix.
;

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
T1A O1A 1.6163(12) . ?
T1A O7A 1.6181(8) . ?
T1A O6A 1.6346(13) . ?
T1A O5A 1.6364(12) . ?
T2A O4A 1.5924(12) . ?
T2A O2A 1.6188(12) . ?
T2A O5A 1.6512(13) 1_556 ?
T2A O6A 1.6655(13) . ?
M1A O3A 2.0542(10) 5_556 ?
M1A O3A 2.0542(10) . ?
M1A O1A 2.0606(12) 6_556 ?
M1A O1A 2.0606(12) . ?
M1A O2A 2.0610(12) 6_556 ?
M2A O4A 2.0154(13) 7_556 ?
M2A O4A 2.0154(13) 4_454 ?
M2A O2A 2.0836(12) 6_556 ?
M2A O2A 2.0836(12) 1_554 ?
M2A O1A 2.1461(13) 6 ?
M2A O1A 2.1461(13) . ?
M3A O3A 2.0190(14) 5_556 ?
M3A O3A 2.0190(14) 1_554 ?
M3A O1A 2.0573(11) . ?
M3A O1A 2.0573(11) 5 ?
M3A O1A 2.0573(11) 2 ?
M3A O1A 2.0573(11) 6 ?
M4A O4A 2.2980(13) 4_455 ?
M4A O4A 2.2980(13) 7_556 ?
M4A O2A 2.4039(13) 6_556 ?
M4A O2A 2.4039(13) . ?
M4A O6A 2.5199(13) 7_556 ?
M4A O6A 2.5199(13) 4_455 ?
M4A O5A 2.7526(14) 7_556 ?
M4A O5A 2.7526(14) 4_455 ?
AM O7A 2.43(2) 3_455 ?
AM O7A 2.61(2) 7 ?
AM O6A 2.705(12) 8_556 ?
AM O6A 2.705(12) 7_556 ?
AM O5A 2.963(11) 7 ?
AM O5A 2.963(11) 8 ?
AM O7A 3.06(2) 7_556 ?
AM O5A 3.118(12) 4_455 ?
AM O5A 3.118(12) 3_455 ?
A2 O7A 2.464(4) 3_455 ?
A2 O7A 2.464(4) 7 ?
A2 O5A 2.65(2) 4_455 ?
A2 O5A 2.65(2) 7 ?
A2 O6A 2.896(14) 4_454 ?
A2 O6A 2.896(14) 7_556 ?
M42 O2A 2.023(12) 6_556 ?
M42 O2A 2.023(12) . ?
M42 O4A 2.2513(13) 4_455 ?
M42 O4A 2.2513(13) 7_556 ?
M42 O6A 2.914(14) 7_556 ?
M42 O6A 2.914(14) 4_455 ?
M42 O5A 3.069(12) 7_556 ?
M42 O5A 3.069(12) 4_455 ?

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

```

fluoro-tremolite 1082\_751\_361.cif

```

_geom_angle_site_symmetry_3
_geom_angle_publ_flag
01A T1A 07A 110.83(7) . . ?
01A T1A 06A 110.96(6) . . ?
07A T1A 06A 109.21(8) . . ?
01A T1A 05A 111.86(6) . . ?
07A T1A 05A 108.55(7) . . ?
06A T1A 05A 105.24(7) . . ?
04A T2A 02A 117.09(6) . . ?
04A T2A 05A 109.28(6) . 1_556 ?
02A T2A 05A 109.26(6) . 1_556 ?
04A T2A 06A 103.21(6) . . ?
02A T2A 06A 108.30(6) . . ?
05A T2A 06A 109.38(7) 1_556 . ?
03A M1A 03A 78.74(6) 5_556 . ?
03A M1A 01A 95.43(5) 5_556 6_556 ?
03A M1A 01A 82.03(5) . 6_556 ?
03A M1A 01A 82.03(5) 5_556 . ?
03A M1A 01A 95.43(5) . . ?
01A M1A 01A 176.73(8) 6_556 . ?
03A M1A 02A 174.64(5) 5_556 . ?
03A M1A 02A 96.49(5) . . ?
01A M1A 02A 86.24(5) 6_556 . ?
01A M1A 02A 96.11(5) . . ?
03A M1A 02A 96.49(5) 5_556 6_556 ?
03A M1A 02A 174.64(5) . 6_556 ?
01A M1A 02A 96.11(5) 6_556 6_556 ?
01A M1A 02A 86.24(5) . 6_556 ?
02A M1A 02A 88.38(7) . 6_556 ?
04A M2A 04A 95.57(8) 7_556 4_454 ?
04A M2A 02A 93.06(5) 7_556 6_556 ?
04A M2A 02A 91.02(5) 4_454 6_556 ?
04A M2A 02A 91.02(5) 7_556 1_554 ?
04A M2A 02A 93.06(5) 4_454 1_554 ?
02A M2A 02A 173.93(7) 6_556 1_554 ?
04A M2A 01A 170.41(5) 7_556 6 ?
04A M2A 01A 92.59(5) 4_454 6 ?
02A M2A 01A 91.82(5) 6_556 6 ?
02A M2A 01A 83.51(5) 1_554 6 ?
04A M2A 01A 92.59(5) 7_556 . ?
04A M2A 01A 170.41(5) 4_454 . ?
02A M2A 01A 83.51(5) 6_556 . ?
02A M2A 01A 91.82(5) 1_554 . ?
01A M2A 01A 79.76(6) 6 . ?
03A M3A 03A 180.0 5_556 1_554 ?
03A M3A 01A 82.97(4) 5_556 . ?
03A M3A 01A 97.03(4) 1_554 . ?
03A M3A 01A 97.03(4) 5_556 5 ?
03A M3A 01A 82.97(4) 1_554 5 ?
01A M3A 01A 180.0 . 5 ?
03A M3A 01A 82.97(4) 5_556 2 ?
03A M3A 01A 97.03(4) 1_554 2 ?
01A M3A 01A 96.04(6) . 2 ?
01A M3A 01A 83.96(6) 5 2 ?
03A M3A 01A 97.03(4) 5_556 6 ?
03A M3A 01A 82.97(4) 1_554 6 ?
01A M3A 01A 83.96(6) . 6 ?
01A M3A 01A 96.04(6) 5 6 ?
01A M3A 01A 180.0 2 6 ?
04A M4A 04A 156.76(7) 4_455 7_556 ?
04A M4A 02A 82.93(5) 4_455 6_556 ?
04A M4A 02A 78.47(4) 7_556 6_556 ?
04A M4A 02A 78.47(4) 4_455 . ?
04A M4A 02A 82.93(5) 7_556 . ?
02A M4A 02A 73.49(6) 6_556 . ?
04A M4A 06A 137.79(5) 4_455 7_556 ?
04A M4A 06A 63.82(4) 7_556 7_556 ?
02A M4A 06A 138.11(4) 6_556 7_556 ?
02A M4A 06A 116.62(4) . 7_556 ?
04A M4A 06A 63.82(4) 4_455 4_455 ?
04A M4A 06A 137.79(5) 7_556 4_455 ?
02A M4A 06A 116.62(4) 6_556 4_455 ?
02A M4A 06A 138.11(4) . 4_455 ?
06A M4A 06A 83.91(6) 7_556 4_455 ?
04A M4A 05A 83.93(4) 4_455 7_556 ?
04A M4A 05A 109.66(4) 7_556 7_556 ?
02A M4A 05A 159.72(4) 6_556 7_556 ?
02A M4A 05A 88.88(4) . 7_556 ?
06A M4A 05A 58.87(4) 7_556 7_556 ?
06A M4A 05A 70.43(4) 4_455 7_556 ?
04A M4A 05A 109.66(4) 4_455 4_455 ?
04A M4A 05A 83.93(4) 7_556 4_455 ?
02A M4A 05A 88.88(4) 6_556 4_455 ?
02A M4A 05A 159.72(4) . 4_455 ?
06A M4A 05A 70.43(4) 7_556 4_455 ?
06A M4A 05A 58.87(4) 4_455 4_455 ?
05A M4A 05A 110.11(6) 7_556 4_455 ?
07A AM 07A 149.8(9) 3_455 7 ?
07A AM 06A 90.5(5) 3_455 8_556 ?
07A AM 06A 107.4(5) 7 8_556 ?
07A AM 06A 90.5(5) 3_455 7_556 ?
07A AM 06A 107.4(5) 7 7_556 ?
06A AM 06A 104.6(7) 8_556 7_556 ?
07A AM 05A 122.7(3) 3_455 7 ?
07A AM 05A 56.2(3) 7 7 ?
06A AM 05A 139.0(7) 8_556 7 ?

```

fluoro-tremolite 1082\_751\_361.cif

06A AM 05A 56.8(2) 7\_556 7 ?  
 07A AM 05A 122.7(3) 3\_455 8 ?  
 07A AM 05A 56.2(3) 7 8 ?  
 06A AM 05A 56.8(2) 8\_556 8 ?  
 06A AM 05A 139.0(7) 7\_556 8 ?  
 05A AM 05A 110.7(6) 7 8 ?  
 07A AM 07A 73.5(5) 3\_455 7\_556 ?  
 07A AM 07A 136.7(7) 7 7\_556 ?  
 06A AM 07A 54.3(3) 8\_556 7\_556 ?  
 06A AM 07A 54.3(3) 7\_556 7\_556 ?  
 05A AM 07A 108.9(4) 7 7\_556 ?  
 05A AM 07A 108.9(4) 8 7\_556 ?  
 07A AM 05A 55.2(3) 3\_455 4\_455 ?  
 07A AM 05A 111.5(5) 7 4\_455 ?  
 06A AM 05A 141.0(7) 8\_556 4\_455 ?  
 06A AM 05A 62.6(2) 7\_556 4\_455 ?  
 05A AM 05A 67.7(2) 7 4\_455 ?  
 05A AM 05A 155.0(7) 8 4\_455 ?  
 07A AM 05A 94.5(4) 7\_556 4\_455 ?  
 07A AM 05A 55.2(3) 3\_455 3\_455 ?  
 07A AM 05A 111.5(5) 7 3\_455 ?  
 06A AM 05A 62.6(2) 8\_556 3\_455 ?  
 06A AM 05A 141.0(7) 7\_556 3\_455 ?  
 05A AM 05A 155.0(7) 7 3\_455 ?  
 05A AM 05A 67.7(2) 8 3\_455 ?  
 07A AM 05A 94.5(4) 7\_556 3\_455 ?  
 05A AM 05A 102.8(6) 4\_455 3\_455 ?  
 07A A2 07A 161.5(11) 3\_455 7 ?  
 07A A2 05A 62.0(2) 3\_455 4\_455 ?  
 07A A2 05A 135.8(8) 7 4\_455 ?  
 07A A2 05A 135.8(8) 3\_455 7 ?  
 07A A2 05A 62.0(2) 7 ?  
 05A A2 05A 79.4(7) 4\_455 7 ?  
 07A A2 06A 105.8(3) 3\_455 4\_454 ?  
 07A A2 06A 85.5(3) 7 4\_454 ?  
 05A A2 06A 58.2(4) 4\_455 4\_454 ?  
 05A A2 06A 66.4(4) 7 4\_454 ?  
 07A A2 06A 85.5(3) 3\_455 7\_556 ?  
 07A A2 06A 105.8(3) 7 7\_556 ?  
 05A A2 06A 66.4(4) 4\_455 7\_556 ?  
 05A A2 06A 58.2(4) 7 7\_556 ?  
 06A A2 06A 105.9(8) 4\_454 7\_556 ?  
 02A M42 02A 90.5(7) 6\_556 . ?  
 02A M42 04A 93.4(3) 6\_556 4\_455 ?  
 02A M42 04A 88.1(3) . 4\_455 ?  
 02A M42 04A 88.1(3) 6\_556 7\_556 ?  
 02A M42 04A 93.4(7) . 7\_556 ?  
 04A M42 04A 177.9(9) 4\_455 7\_556 ?  
 02A M42 06A 136.6(2) 6\_556 7\_556 ?  
 02A M42 06A 115.0(2) . 7\_556 ?  
 04A M42 06A 120.5(6) 4\_455 7\_556 ?  
 04A M42 06A 57.6(3) 7\_556 7\_556 ?  
 02A M42 06A 115.0(2) 6\_556 4\_455 ?  
 02A M42 06A 136.6(2) . 4\_455 ?  
 04A M42 06A 57.6(3) 4\_455 4\_455 ?  
 04A M42 06A 120.5(6) 7\_556 4\_455 ?  
 06A M42 06A 70.7(4) 7\_556 4\_455 ?  
 02A M42 05A 170.93(12) 6\_556 7\_556 ?  
 02A M42 05A 88.10(12) . 7\_556 ?  
 04A M42 05A 77.6(3) 4\_455 7\_556 ?  
 04A M42 05A 101.0(4) 7\_556 7\_556 ?  
 06A M42 05A 51.4(2) 7\_556 7\_556 ?  
 06A M42 05A 61.2(3) 4\_455 7\_556 ?  
 02A M42 05A 88.10(12) 6\_556 4\_455 ?  
 02A M42 05A 170.93(12) . 4\_455 ?  
 04A M42 05A 101.0(4) 4\_455 4\_455 ?  
 04A M42 05A 77.6(3) 7\_556 4\_455 ?  
 06A M42 05A 61.2(3) 7\_556 4\_455 ?  
 06A M42 05A 51.4(2) 4\_455 4\_455 ?  
 05A M42 05A 94.7(5) 7\_556 4\_455 ?  
 T1A 05A T2A 136.32(7) . 1\_554 ?  
 T1A 06A T2A 138.40(7) . ?  
 T1A 07A T1A 137.66(11) . 2 ?  
 05A 06A 05A 167.09(7) . 1\_556 ?  
 06A 07A 06A 107.64(8) . 2 ?

\_refine\_diff\_density\_max 0.61  
 \_refine\_diff\_density\_min -0.35

loop\_  
 \_refln\_index\_h  
 \_refln\_index\_k  
 \_refln\_index\_l  
 \_refln\_F\_meas  
 \_refln\_F\_sigma  
 0 2 0 102.1 0.7  
 0 4 0 316.6 0.9  
 0 6 0 16.4 3.8  
 0 8 0 102.9 1.4  
 0 10 0 235.4 1.5  
 0 12 0 785.8 1.6  
 0 14 0 19.1 13.8  
 0 16 0 23.8 4.9  
 0 18 0 56.3 2.7  
 0 20 0 273.6 2.3  
 0 22 0 276.3 2.5

## fluoro-tremolite 1082\_751\_361.cif

0	24	0	393.2	2.6
1	1	0	198.8	0.8
1	3	0	145.3	1.3
1	5	0	0.0	7.8
1	7	0	16.1	4.3
1	9	0	268.8	3.1
1	11	0	520.3	2.5
1	13	0	45.7	1.8
1	15	0	20.2	8.2
1	17	0	14.1	13.9
1	19	0	7.7	15.9
1	21	0	88.8	8.9
1	23	0	55.7	6.5
1	25	0	54.7	5.7
2	0	0	109.2	0.9
2	2	0	118.2	2.1
2	4	0	429.8	0.9
2	6	0	31.9	5.0
2	8	0	104.4	2.8
2	10	0	114.3	1.1
2	12	0	152.0	1.4
2	14	0	95.3	4.9
2	16	0	4.1	11.7
2	18	0	110.8	2.4
2	20	0	65.1	2.3
2	22	0	89.9	2.1
2	24	0	157.9	4.8
3	1	0	573.4	3.5
3	3	0	258.5	1.1
3	5	0	247.9	2.4
3	7	0	303.3	3.1
3	9	0	79.4	1.6
3	11	0	361.2	2.4
3	13	0	18.8	7.8
3	15	0	26.0	20.1
3	17	0	69.2	1.9
3	19	0	115.3	5.4
3	21	0	19.6	12.1
3	23	0	165.6	4.4
4	0	0	28.0	2.2
4	2	0	73.9	1.6
4	4	0	45.0	3.2
4	6	0	69.9	1.5
4	8	0	396.2	7.9
4	10	0	177.9	5.8
4	12	0	163.4	3.8
4	14	0	29.1	4.9
4	16	0	251.4	1.8
4	18	0	67.6	2.3
4	20	0	187.1	4.2
4	22	0	160.5	4.8
4	24	0	17.3	12.2
5	1	0	379.6	3.8
5	3	0	256.4	2.3
5	5	0	60.5	1.4
5	7	0	151.6	1.2
5	9	0	42.6	2.2
5	11	0	132.1	2.0
5	13	0	271.3	3.6
5	15	0	163.0	1.9
5	17	0	18.5	11.2
5	19	0	49.8	6.9
5	21	0	158.0	3.9
5	23	0	208.5	6.2
6	0	0	448.6	1.6
6	2	0	171.7	3.2
6	4	0	5.3	11.9
6	6	0	23.4	18.0
6	8	0	189.7	1.3
6	10	0	35.2	11.4
6	12	0	56.8	3.7
6	14	0	7.6	12.7
6	16	0	46.2	7.2
6	18	0	102.1	2.0
6	20	0	58.0	5.9
6	22	0	86.0	3.4
7	1	0	281.9	2.5
7	3	0	156.7	1.9
7	5	0	59.2	4.1
7	7	0	134.4	1.5
7	9	0	391.8	4.4
7	11	0	579.0	4.4
7	13	0	164.3	2.7
7	15	0	209.6	1.8
7	17	0	47.1	3.5
7	19	0	113.8	7.8
7	21	0	45.6	3.9
8	0	0	410.1	1.9
8	2	0	96.3	1.6
8	4	0	87.8	3.7
8	6	0	107.2	1.8
8	8	0	59.3	3.4
8	10	0	72.0	2.1
8	12	0	143.0	1.9
8	14	0	30.4	13.7
8	16	0	5.2	15.7

## fluoro-tremolite 1082\_751\_361.cif

8	18	0	8.9	17.8
8	20	0	38.4	4.0
9	1	0	99.1	3.3
9	3	0	73.2	2.0
9	5	0	6.6	14.0
9	7	0	237.2	1.6
9	9	0	60.8	2.4
9	11	0	86.8	2.4
9	13	0	79.6	5.1
9	15	0	135.4	4.0
9	17	0	69.5	2.8
10	0	0	360.1	2.2
10	2	0	44.0	2.9
10	4	0	16.2	18.5
10	6	0	32.8	11.8
10	8	0	241.8	4.2
10	10	0	124.5	1.8
10	12	0	310.3	3.1
10	14	0	0.0	12.3
10	16	0	164.1	2.0
11	1	0	226.8	6.4
11	3	0	35.4	7.0
11	5	0	110.9	4.0
11	7	0	26.2	12.5
11	9	0	55.5	5.8
11	11	0	250.2	2.8
11	13	0	61.5	2.9
12	0	0	66.3	3.2
12	2	0	11.9	20.0
12	4	0	112.8	2.8
12	6	0	20.2	21.5
12	8	0	161.2	2.1
12	10	0	71.8	2.5
13	1	0	101.7	5.8
13	3	0	50.9	15.9
13	5	0	46.7	3.6
0	0	1	130.0	0.9
0	2	1	57.8	8.0
0	4	1	41.5	1.6
0	6	1	503.1	1.1
0	8	1	76.1	4.9
0	10	1	202.1	2.4
0	12	1	104.2	7.8
0	14	1	138.2	6.7
0	16	1	207.6	2.5
0	18	1	26.5	10.3
0	20	1	36.1	5.4
0	22	1	5.7	14.4
0	24	1	0.0	12.7
1	1	1	113.7	0.9
-1	1	1	238.9	3.0
1	3	1	479.1	2.0
-1	3	1	287.6	4.0
1	5	1	777.7	2.2
-1	5	1	218.9	2.5
1	7	1	249.8	3.2
-1	7	1	432.9	4.9
1	9	1	109.8	4.4
-1	9	1	408.3	4.1
1	11	1	82.1	4.9
-1	11	1	31.3	4.3
1	13	1	142.7	6.3
-1	13	1	214.1	2.0
1	15	1	253.0	1.6
-1	15	1	174.5	2.8
1	17	1	532.7	1.4
-1	17	1	179.1	7.7
1	19	1	186.4	6.9
-1	19	1	123.3	1.9
1	21	1	233.2	1.8
-1	21	1	92.8	6.5
1	23	1	20.6	22.5
-1	23	1	84.8	2.1
1	25	1	130.1	4.7
-1	25	1	18.7	18.4
2	0	1	137.5	1.1
-2	0	1	127.6	1.0
2	2	1	481.5	2.1
-2	2	1	39.2	3.8
2	4	1	46.2	2.7
-2	4	1	70.1	1.1
2	6	1	601.5	4.4
-2	6	1	216.9	2.7
2	8	1	5.9	12.4
-2	8	1	26.1	4.7
2	10	1	176.4	5.7
-2	10	1	69.4	5.0
2	12	1	63.6	4.0
-2	12	1	72.6	2.8
2	14	1	122.0	6.3
-2	14	1	282.4	1.3
2	16	1	185.9	2.8
-2	16	1	193.1	2.4
2	18	1	0.0	11.1
-2	18	1	71.7	3.0
2	20	1	64.4	2.5

## fluoro-tremolite 1082\_751\_361.cif

-2	20	1	37.7	4.0
2	22	1	66.3	5.2
-2	22	1	148.2	2.0
2	24	1	25.4	14.1
-2	24	1	36.5	12.4
3	1	1	101.3	1.3
-3	1	1	126.2	0.8
3	3	1	97.8	3.4
-3	3	1	398.7	1.0
3	5	1	435.4	1.6
-3	5	1	529.5	4.9
3	7	1	41.5	2.7
-3	7	1	132.9	3.0
3	9	1	73.0	1.5
-3	9	1	187.0	3.9
3	11	1	52.5	22.4
-3	11	1	200.6	2.9
3	13	1	182.3	3.3
-3	13	1	11.9	11.0
3	15	1	38.8	4.2
-3	15	1	124.6	3.6
3	17	1	99.8	9.4
-3	17	1	264.8	4.3
3	19	1	9.0	17.4
-3	19	1	59.5	4.3
3	21	1	17.9	18.1
-3	21	1	91.3	3.3
3	23	1	95.6	4.2
-3	23	1	80.8	2.6
4	0	1	95.9	1.5
-4	0	1	147.3	1.3
4	2	1	139.6	1.2
-4	2	1	382.9	2.0
4	4	1	15.1	10.3
-4	4	1	76.6	1.9
4	6	1	747.5	2.3
-4	6	1	145.8	5.2
4	8	1	61.3	8.6
-4	8	1	17.4	7.9
4	10	1	98.7	4.0
-4	10	1	157.8	5.8
4	12	1	58.0	2.0
-4	12	1	0.0	38.4
4	14	1	390.9	1.4
-4	14	1	41.2	5.4
4	16	1	274.6	2.5
-4	16	1	149.5	5.9
4	18	1	382.7	2.9
-4	18	1	80.2	1.9
4	20	1	7.7	12.7
-4	20	1	62.1	2.6
4	22	1	152.5	3.3
-4	22	1	0.0	12.1
-4	24	1	28.3	8.2
5	1	1	47.7	3.5
-5	1	1	68.4	1.7
5	3	1	11.6	11.6
-5	3	1	88.1	1.9
5	5	1	357.6	1.2
-5	5	1	147.6	1.1
5	7	1	98.4	2.5
-5	7	1	166.2	3.8
5	9	1	114.0	6.6
-5	9	1	145.6	2.6
5	11	1	87.4	3.1
-5	11	1	21.2	9.2
5	13	1	72.1	3.2
-5	13	1	75.0	1.6
5	15	1	55.7	3.2
-5	15	1	47.6	17.8
5	17	1	151.3	8.1
-5	17	1	77.0	7.1
5	19	1	46.5	4.5
-5	19	1	28.2	9.9
5	21	1	10.7	19.2
-5	21	1	55.7	4.0
-5	23	1	58.1	3.2
6	0	1	59.4	2.2
-6	0	1	90.2	1.7
6	2	1	210.4	5.1
-6	2	1	96.6	2.6
6	4	1	0.0	9.8
-6	4	1	36.3	2.4
6	6	1	344.6	5.0
-6	6	1	962.8	6.9
6	8	1	33.6	4.4
-6	8	1	118.9	1.4
6	10	1	33.5	3.9
-6	10	1	178.5	3.0
6	12	1	96.5	4.1
-6	12	1	70.0	2.4
6	14	1	91.6	6.1
-6	14	1	187.4	2.0
6	16	1	88.8	2.5
-6	16	1	215.1	2.0
6	18	1	373.0	5.0

## fluoro-tremolite 1082\_751\_361.cif

-6	18	1	315.5	4.0
6	20	1	119.2	2.2
-6	20	1	27.3	7.8
-6	22	1	17.3	14.7
7	1	1	24.4	3.6
-7	1	1	21.0	5.6
7	3	1	150.9	3.0
-7	3	1	90.5	4.8
7	5	1	136.5	2.8
-7	5	1	509.9	4.0
7	7	1	84.9	4.5
-7	7	1	197.8	1.3
7	9	1	18.9	6.2
-7	9	1	67.0	2.4
7	11	1	10.3	15.5
-7	11	1	42.2	2.7
7	13	1	18.0	19.8
-7	13	1	26.2	21.7
7	15	1	109.5	7.0
-7	15	1	45.3	4.3
7	17	1	134.6	4.0
-7	17	1	341.1	4.4
7	19	1	4.4	14.0
-7	19	1	143.1	3.5
-7	21	1	68.1	5.0
8	0	1	94.1	2.2
-8	0	1	45.1	2.8
8	2	1	57.7	2.6
-8	2	1	194.1	1.4
8	4	1	26.9	3.0
-8	4	1	16.5	10.5
8	6	1	424.4	3.6
-8	6	1	127.8	1.7
8	8	1	44.5	4.1
-8	8	1	52.0	2.7
8	10	1	115.2	4.7
-8	10	1	75.9	3.7
8	12	1	9.8	18.5
-8	12	1	67.7	2.1
8	14	1	128.4	1.9
-8	14	1	5.7	13.8
8	16	1	151.6	2.0
-8	16	1	136.7	2.0
8	18	1	104.3	5.6
-8	18	1	181.9	2.2
-8	20	1	90.2	4.0
9	1	1	22.5	4.8
-9	1	1	56.0	2.3
9	3	1	16.2	18.6
-9	3	1	90.5	1.7
9	5	1	13.5	12.4
-9	5	1	246.9	2.2
9	7	1	147.3	4.1
-9	7	1	38.2	11.0
9	9	1	98.6	2.6
-9	9	1	20.8	21.1
9	11	1	76.7	2.6
-9	11	1	28.6	11.5
9	13	1	68.4	5.2
-9	13	1	195.8	2.5
9	15	1	27.1	13.2
-9	15	1	6.1	14.3
9	17	1	57.9	23.5
-9	17	1	78.6	5.3
-9	19	1	25.6	10.0
10	0	1	0.0	16.9
-10	0	1	58.6	2.7
10	2	1	118.5	1.8
-10	2	1	57.4	3.2
10	4	1	107.4	2.0
-10	4	1	41.2	5.1
10	6	1	97.3	2.0
-10	6	1	298.6	2.9
10	8	1	88.7	3.1
-10	8	1	19.2	11.8
10	10	1	71.1	4.0
-10	10	1	62.7	3.0
10	12	1	53.5	3.8
-10	12	1	29.8	8.4
10	14	1	47.9	3.2
-10	14	1	207.7	2.9
-10	16	1	191.1	5.4
11	1	1	0.0	11.7
-11	1	1	0.0	11.4
11	3	1	190.2	2.5
-11	3	1	38.3	6.9
11	5	1	408.2	2.4
-11	5	1	63.4	6.8
11	7	1	215.3	4.3
-11	7	1	176.8	4.5
11	9	1	99.6	2.2
-11	9	1	138.8	1.9
11	11	1	47.9	3.8
-11	11	1	83.4	2.4
-11	13	1	36.1	20.0
-11	15	1	44.5	11.7

## fluoro-tremolite 1082\_751\_361.cif

12	0	1	102.1	2.9
-12	0	1	33.3	6.4
12	2	1	25.4	9.6
-12	2	1	147.4	2.8
12	4	1	55.0	3.1
-12	4	1	104.4	2.1
12	6	1	183.3	2.6
-12	6	1	29.0	15.1
12	8	1	22.2	9.1
-12	8	1	77.9	3.9
-12	10	1	40.5	9.8
-12	12	1	65.8	3.8
-13	1	1	22.5	22.3
-13	3	1	161.2	2.1
-13	5	1	249.5	2.9
-13	7	1	73.2	7.5
0	0	2	411.2	1.2
0	2	2	127.3	1.0
0	4	2	35.7	4.0
0	6	2	31.2	2.6
0	8	2	163.0	7.3
0	10	2	47.2	4.3
0	12	2	510.5	5.3
0	14	2	94.5	4.0
0	16	2	14.8	16.6
0	18	2	100.3	2.1
0	20	2	0.0	11.9
0	22	2	55.6	6.3
0	24	2	250.0	4.6
1	1	2	0.0	8.7
-1	1	2	30.1	2.7
1	3	2	121.2	4.6
-1	3	2	33.2	1.9
1	5	2	72.5	7.0
-1	5	2	182.4	1.9
1	7	2	84.8	5.2
-1	7	2	252.6	3.5
1	9	2	333.3	2.0
-1	9	2	13.9	12.2
1	11	2	509.2	3.6
-1	11	2	52.5	3.8
1	13	2	101.9	4.0
-1	13	2	172.5	2.2
1	15	2	132.3	6.4
-1	15	2	131.2	6.0
1	17	2	16.8	19.5
-1	17	2	19.5	11.2
1	19	2	60.3	3.2
-1	19	2	34.1	12.5
1	21	2	36.5	8.1
-1	21	2	111.6	5.7
1	23	2	96.2	3.0
-1	23	2	55.4	4.7
2	0	2	622.4	1.4
-2	0	2	910.4	1.2
2	2	2	122.8	1.5
-2	2	2	144.8	2.0
2	4	2	237.5	2.4
-2	4	2	283.2	6.1
2	6	2	43.0	3.2
-2	6	2	58.0	3.0
2	8	2	44.3	4.7
-2	8	2	378.8	5.6
2	10	2	113.2	8.0
-2	10	2	209.0	3.7
2	12	2	90.1	6.6
-2	12	2	738.5	9.3
2	14	2	38.8	3.2
-2	14	2	36.3	2.3
2	16	2	94.2	1.8
-2	16	2	196.7	1.6
2	18	2	40.3	6.9
-2	18	2	76.9	4.8
2	20	2	191.1	8.9
-2	20	2	187.3	8.0
2	22	2	163.2	9.4
-2	22	2	206.7	6.4
-2	24	2	232.2	9.2
3	1	2	124.8	1.2
-3	1	2	431.4	3.2
3	3	2	120.5	2.2
-3	3	2	216.5	4.9
3	5	2	85.9	4.2
-3	5	2	238.4	7.2
3	7	2	170.9	7.6
-3	7	2	172.3	2.6
3	9	2	4.8	10.3
-3	9	2	145.8	2.0
3	11	2	15.2	10.6
-3	11	2	354.3	5.8
3	13	2	211.3	2.2
-3	13	2	20.9	6.5
3	15	2	122.7	6.8
-3	15	2	21.0	15.9
3	17	2	5.6	15.0
-3	17	2	16.5	15.5

## fluoro-tremolite 1082\_751\_361.cif

3	19	2	27.0	10.6
-3	19	2	79.5	4.2
3	21	2	113.6	3.2
-3	21	2	35.5	6.2
3	23	2	122.6	2.1
-3	23	2	111.3	3.5
4	0	2	518.8	1.6
-4	0	2	527.5	1.4
4	2	2	148.4	1.2
-4	2	2	112.6	1.9
4	4	2	323.2	1.5
-4	4	2	280.6	1.8
4	6	2	22.0	10.1
-4	6	2	24.7	6.8
4	8	2	81.3	4.7
-4	8	2	295.9	4.1
4	10	2	91.8	5.7
-4	10	2	90.6	1.7
4	12	2	393.1	3.0
-4	12	2	21.3	8.0
4	14	2	26.1	4.3
-4	14	2	75.2	4.1
4	16	2	56.6	6.3
-4	16	2	70.4	7.1
4	18	2	187.7	9.4
-4	18	2	88.9	2.2
4	20	2	8.7	18.0
-4	20	2	75.9	3.5
4	22	2	116.8	10.3
-4	22	2	191.1	2.1
5	1	2	645.6	2.3
-5	1	2	337.7	2.2
5	3	2	321.8	2.8
-5	3	2	57.7	2.9
5	5	2	188.4	2.8
-5	5	2	87.4	4.6
5	7	2	76.5	3.3
-5	7	2	14.9	16.4
5	9	2	227.9	1.5
-5	9	2	291.4	3.5
5	11	2	558.1	3.7
-5	11	2	638.1	4.0
5	13	2	172.2	6.5
-5	13	2	198.6	1.5
5	15	2	86.8	5.7
-5	15	2	111.2	2.3
5	17	2	10.4	18.3
-5	17	2	20.4	18.5
5	19	2	159.2	9.9
-5	19	2	31.6	8.8
5	21	2	37.4	7.1
-5	21	2	42.9	9.9
-5	23	2	192.0	4.0
6	0	2	250.6	2.0
-6	0	2	724.9	1.6
6	2	2	14.6	10.7
-6	2	2	41.1	31.2
6	4	2	111.4	2.5
-6	4	2	281.9	1.7
6	6	2	90.4	3.4
-6	6	2	22.8	6.6
6	8	2	32.9	5.8
-6	8	2	135.1	3.3
6	10	2	123.7	5.1
-6	10	2	178.1	3.0
6	12	2	69.3	5.8
-6	12	2	287.6	1.5
6	14	2	58.7	4.1
-6	14	2	53.5	6.2
6	16	2	33.0	7.1
-6	16	2	131.9	3.2
6	18	2	33.6	5.1
-6	18	2	55.9	5.0
6	20	2	36.0	7.5
-6	20	2	254.9	1.9
-6	22	2	200.6	4.1
7	1	2	81.3	2.4
-7	1	2	148.8	1.3
7	3	2	237.1	1.6
-7	3	2	226.6	1.6
7	5	2	108.1	4.6
-7	5	2	44.3	8.7
7	7	2	130.8	6.0
-7	7	2	167.9	2.6
7	9	2	31.8	4.7
-7	9	2	81.3	3.7
7	11	2	105.8	3.1
-7	11	2	40.5	4.1
7	13	2	51.0	6.7
-7	13	2	171.4	3.9
7	15	2	95.9	3.1
-7	15	2	164.5	3.5
7	17	2	38.4	7.8
-7	17	2	11.5	19.4
7	19	2	94.8	2.7
-7	19	2	55.0	4.0

## fluoro-tremolite 1082\_751\_361.cif

-7	21	2	163.2	8.5
8	0	2	442.3	2.2
-8	0	2	124.0	2.0
8	2	2	24.2	9.6
-8	2	2	71.1	2.2
8	4	2	187.4	2.1
-8	4	2	243.5	1.4
8	6	2	51.9	2.3
-8	6	2	37.2	12.4
8	8	2	75.2	4.0
-8	8	2	18.2	13.3
8	10	2	106.7	1.9
-8	10	2	64.5	2.5
8	12	2	89.0	5.3
-8	12	2	84.4	3.4
8	14	2	39.8	12.1
-8	14	2	52.1	4.6
8	16	2	72.0	3.0
-8	16	2	66.4	4.8
-8	18	2	129.9	2.2
-8	20	2	11.8	20.9
9	1	2	55.8	3.2
-9	1	2	257.1	3.7
9	3	2	0.0	11.9
-9	3	2	254.0	1.5
9	5	2	83.4	6.8
-9	5	2	191.9	2.1
9	7	2	44.5	4.6
-9	7	2	42.7	18.0
9	9	2	80.2	3.1
-9	9	2	199.4	2.2
9	11	2	176.4	1.9
-9	11	2	246.7	6.6
9	13	2	16.9	16.5
-9	13	2	0.0	11.8
9	15	2	16.7	13.8
-9	15	2	70.5	2.3
-9	17	2	2.5	12.7
-9	19	2	150.8	4.4
10	0	2	170.7	2.5
-10	0	2	191.9	2.2
10	2	2	46.3	7.6
-10	2	2	101.2	3.8
10	4	2	215.8	2.2
-10	4	2	124.9	1.7
10	6	2	7.1	18.9
-10	6	2	181.9	3.2
10	8	2	111.4	2.4
-10	8	2	30.0	6.2
10	10	2	27.4	11.7
-10	10	2	39.4	9.0
10	12	2	157.8	3.6
-10	12	2	66.7	2.8
-10	14	2	19.9	13.8
-10	16	2	27.4	16.7
11	1	2	53.1	3.0
-11	1	2	107.8	4.6
11	3	2	107.8	4.9
-11	3	2	139.1	3.9
11	5	2	46.9	4.5
-11	5	2	52.1	3.0
11	7	2	116.2	2.7
-11	7	2	100.9	2.1
11	9	2	79.7	3.4
-11	9	2	23.6	12.4
-11	11	2	64.0	4.2
-11	13	2	93.9	4.0
-11	15	2	57.2	3.3
-12	0	2	471.3	2.5
-12	2	2	110.2	2.2
-12	4	2	127.8	3.1
-12	6	2	0.0	12.3
-12	8	2	53.2	19.8
-12	10	2	31.0	9.7
-12	12	2	163.5	2.0
-13	1	2	217.7	2.3
-13	3	2	36.5	7.5
-13	5	2	53.7	4.7
-13	7	2	18.6	11.9
0	0	3	141.5	1.6
0	2	3	364.3	4.8
0	4	3	6.3	13.7
0	6	3	171.9	9.0
0	8	3	0.0	8.2
0	10	3	173.0	10.4
0	12	3	57.6	4.6
0	14	3	88.6	7.5
0	16	3	137.3	8.0
0	18	3	56.6	7.4
0	20	3	75.4	2.5
0	22	3	24.2	17.0
1	1	3	117.7	2.0
-1	1	3	69.6	1.5
1	3	3	19.4	9.1
-1	3	3	393.2	5.1
1	5	3	123.7	6.3

## fluoro-tremolite 1082\_751\_361.cif

-1	5	3	741.1	8.3
1	7	3	103.8	7.0
-1	7	3	347.7	1.5
1	9	3	180.3	10.5
-1	9	3	189.4	2.4
1	11	3	13.2	11.6
-1	11	3	147.8	13.4
1	13	3	75.1	6.8
-1	13	3	8.4	16.6
1	15	3	10.9	20.1
-1	15	3	122.4	6.5
1	17	3	85.9	3.1
-1	17	3	382.6	3.0
1	19	3	8.0	17.1
-1	19	3	115.8	5.5
1	21	3	28.1	12.2
-1	21	3	104.6	2.4
-1	23	3	71.6	3.7
2	0	3	83.5	2.0
-2	0	3	65.7	2.3
2	2	3	230.5	4.2
-2	2	3	49.2	2.8
2	4	3	17.2	11.6
-2	4	3	12.5	11.8
2	6	3	433.0	2.1
-2	6	3	755.8	14.8
2	8	3	57.4	2.4
-2	8	3	50.3	2.3
2	10	3	276.1	4.6
-2	10	3	9.1	17.1
2	12	3	55.9	3.2
-2	12	3	58.3	2.9
2	14	3	253.0	4.8
-2	14	3	234.0	3.6
2	16	3	185.8	9.0
-2	16	3	250.5	4.8
2	18	3	59.3	4.5
-2	18	3	329.9	7.2
2	20	3	0.0	10.0
-2	20	3	23.6	21.4
2	22	3	66.4	3.3
-2	22	3	80.1	14.6
3	1	3	4.6	12.2
-3	1	3	142.5	2.0
3	3	3	40.5	2.2
-3	3	3	126.4	2.2
3	5	3	110.7	3.1
-3	5	3	123.6	2.4
3	7	3	103.9	5.9
-3	7	3	151.8	1.9
3	9	3	139.1	6.6
-3	9	3	246.3	3.9
3	11	3	50.5	3.2
-3	11	3	0.0	10.9
3	13	3	19.3	16.2
-3	13	3	182.6	4.2
3	15	3	10.7	20.4
-3	15	3	104.2	6.8
3	17	3	56.8	3.5
-3	17	3	4.1	13.0
3	19	3	24.2	19.4
-3	19	3	33.5	4.8
3	21	3	27.0	10.7
-3	21	3	54.0	5.6
-3	23	3	86.0	4.9
4	0	3	14.1	15.4
-4	0	3	57.4	2.2
4	2	3	224.7	3.5
-4	2	3	19.4	10.3
4	4	3	76.6	6.9
-4	4	3	24.1	4.5
4	6	3	278.3	2.2
-4	6	3	150.6	4.1
4	8	3	5.9	13.6
-4	8	3	7.9	14.9
4	10	3	94.9	2.8
-4	10	3	144.0	2.1
4	12	3	65.7	3.7
-4	12	3	85.6	2.2
4	14	3	45.5	9.2
-4	14	3	92.6	2.9
4	16	3	76.2	4.8
-4	16	3	162.7	5.0
4	18	3	266.1	3.3
-4	18	3	123.2	3.2
4	20	3	63.4	2.9
-4	20	3	64.4	3.7
-4	22	3	34.8	5.0
5	1	3	15.2	11.2
-5	1	3	35.9	2.4
5	3	3	251.3	1.9
-5	3	3	222.6	1.8
5	5	3	298.8	5.3
-5	5	3	395.6	5.3
5	7	3	61.8	5.9
-5	7	3	96.2	1.6

## fluoro-tremolite 1082\_751\_361.cif

5	9	3	133.6	4.9
-5	9	3	33.1	7.5
5	11	3	72.6	10.6
-5	11	3	57.8	23.9
5	13	3	32.3	5.4
-5	13	3	94.1	5.5
5	15	3	100.0	4.0
-5	15	3	149.6	4.9
5	17	3	131.9	8.1
-5	17	3	332.0	5.9
5	19	3	6.3	15.7
-5	19	3	119.2	3.2
-5	21	3	154.0	2.0
6	0	3	117.1	2.3
-6	0	3	187.3	2.0
6	2	3	22.9	18.5
-6	2	3	174.1	1.7
6	4	3	24.9	6.0
-6	4	3	23.9	6.8
6	6	3	519.8	1.6
-6	6	3	85.9	2.3
6	8	3	64.5	2.3
-6	8	3	12.1	13.4
6	10	3	34.0	27.7
-6	10	3	26.0	4.2
6	12	3	6.5	14.8
-6	12	3	55.3	2.1
6	14	3	186.5	14.4
-6	14	3	23.7	9.5
6	16	3	159.9	4.2
-6	16	3	117.2	2.1
6	18	3	282.9	2.8
-6	18	3	205.6	6.5
-6	20	3	86.4	4.7
7	1	3	50.3	8.1
-7	1	3	42.8	7.0
7	3	3	37.5	9.4
-7	3	3	16.9	11.0
7	5	3	87.4	2.1
-7	5	3	87.8	3.7
7	7	3	42.3	3.5
-7	7	3	254.0	4.7
7	9	3	135.1	3.2
-7	9	3	119.9	2.1
7	11	3	52.4	5.3
-7	11	3	93.2	1.8
7	13	3	62.4	7.3
-7	13	3	125.4	1.9
7	15	3	47.2	5.6
-7	15	3	50.3	3.0
-7	17	3	144.8	3.8
-7	19	3	132.0	2.5
8	0	3	20.5	16.6
-8	0	3	76.6	2.7
8	2	3	55.0	2.4
-8	2	3	17.2	10.9
8	4	3	42.3	9.5
-8	4	3	76.3	2.9
8	6	3	181.9	9.9
-8	6	3	488.8	1.5
8	8	3	49.9	3.0
-8	8	3	99.9	2.0
8	10	3	0.0	12.8
-8	10	3	4.3	13.1
8	12	3	84.2	7.9
-8	12	3	32.4	4.6
8	14	3	5.1	15.2
-8	14	3	220.8	2.8
-8	16	3	151.0	3.2
-8	18	3	261.9	2.6
9	1	3	10.2	18.6
-9	1	3	36.2	3.9
9	3	3	114.6	2.1
-9	3	3	152.8	5.3
9	5	3	358.2	2.0
-9	5	3	378.1	3.1
9	7	3	158.9	4.9
-9	7	3	135.7	1.9
9	9	3	29.8	10.9
-9	9	3	39.2	3.4
9	11	3	18.6	20.7
-9	11	3	94.9	8.8
-9	13	3	10.1	18.4
-9	15	3	58.9	3.1
-9	17	3	229.3	3.5
10	0	3	63.5	3.5
-10	0	3	71.3	2.7
10	2	3	31.8	8.6
-10	2	3	150.1	2.5
10	4	3	52.9	5.1
-10	4	3	38.9	6.2
10	6	3	46.9	5.7
-10	6	3	22.9	10.2
10	8	3	83.2	3.9
-10	8	3	16.3	19.4
-10	10	3	26.7	7.3

## fluoro-tremolite 1082\_751\_361.cif

-10	12	3	34.5	6.3
-10	14	3	45.6	3.7
-10	16	3	83.3	2.5
-11	1	3	73.1	5.8
-11	3	3	63.4	2.4
-11	5	3	227.2	5.5
-11	7	3	40.2	3.9
-11	9	3	60.8	4.3
-11	11	3	39.0	18.1
-11	13	3	46.6	17.8
-12	0	3	24.8	6.4
-12	2	3	88.7	4.9
-12	4	3	57.2	2.7
-12	6	3	362.8	11.0
-12	8	3	11.9	13.3
-12	10	3	130.5	3.4
-13	1	3	0.0	12.8
-13	3	3	35.7	8.3
-13	5	3	20.3	15.2
-13	7	3	75.1	6.9
0	0	4	525.4	1.8
0	2	4	63.4	2.5
0	4	4	128.0	2.8
0	6	4	53.0	4.3
0	8	4	134.4	4.9
0	10	4	143.6	6.9
0	12	4	382.5	2.0
0	14	4	23.1	10.0
0	16	4	96.5	2.5
0	18	4	62.2	5.7
0	20	4	85.8	8.2
1	1	4	30.8	3.4
-1	1	4	479.6	1.9
1	3	4	142.3	1.4
-1	3	4	266.6	1.5
1	5	4	8.4	16.7
-1	5	4	152.3	9.7
1	7	4	132.8	5.1
-1	7	4	111.2	6.3
1	9	4	0.0	11.2
-1	9	4	183.0	1.5
1	11	4	92.6	3.4
-1	11	4	411.1	3.9
1	13	4	88.0	10.1
-1	13	4	80.1	3.6
1	15	4	92.3	8.3
-1	15	4	48.0	6.5
1	17	4	18.8	15.7
-1	17	4	42.7	4.9
1	19	4	47.3	5.4
-1	19	4	135.2	5.3
-1	21	4	25.4	8.5
2	0	4	652.9	1.9
-2	0	4	237.1	1.9
2	2	4	93.4	1.7
-2	2	4	84.9	2.2
2	4	4	24.7	7.4
-2	4	4	155.3	2.3
2	6	4	25.7	3.7
-2	6	4	33.2	24.9
2	8	4	86.3	6.3
-2	8	4	18.2	18.9
2	10	4	88.1	9.7
-2	10	4	44.0	4.6
2	12	4	198.4	8.1
-2	12	4	230.4	6.3
2	14	4	7.4	16.4
-2	14	4	68.2	7.0
2	16	4	18.0	20.3
-2	16	4	83.5	7.6
2	18	4	77.8	5.9
-2	18	4	92.3	2.2
2	20	4	97.6	5.3
-2	20	4	11.9	22.0
3	1	4	293.3	1.9
-3	1	4	188.0	1.5
3	3	4	34.0	4.3
-3	3	4	220.7	3.0
3	5	4	19.8	20.8
-3	5	4	18.8	19.3
3	7	4	71.1	2.2
-3	7	4	98.4	1.6
3	9	4	224.4	1.6
-3	9	4	7.8	15.6
3	11	4	506.8	6.8
-3	11	4	25.9	4.0
3	13	4	171.7	6.7
-3	13	4	147.6	2.9
3	15	4	107.0	4.2
-3	15	4	91.2	3.0
3	17	4	17.0	12.8
-3	17	4	11.8	20.8
3	19	4	73.2	18.3
-3	19	4	32.8	10.7
-3	21	4	120.5	8.7
4	0	4	52.1	3.4

## fluoro-tremolite 1082\_751\_361.cif

-4	0	4	629.9	1.8
4	2	4	23.5	9.3
-4	2	4	105.3	1.9
4	4	4	74.5	2.0
-4	4	4	223.7	1.9
4	6	4	53.0	3.6
-4	6	4	28.1	5.4
4	8	4	60.0	3.2
-4	8	4	84.5	2.2
4	10	4	76.0	6.5
-4	10	4	97.6	3.8
4	12	4	159.2	7.9
-4	12	4	161.4	6.9
4	14	4	95.3	2.3
-4	14	4	27.5	6.4
4	16	4	45.6	5.1
-4	16	4	89.4	2.4
4	18	4	33.4	13.7
-4	18	4	45.7	6.6
-4	20	4	230.1	3.8
5	1	4	65.0	8.8
-5	1	4	21.4	17.3
5	3	4	75.7	2.3
-5	3	4	13.2	12.7
5	5	4	23.0	18.7
-5	5	4	54.9	2.5
5	7	4	186.8	8.7
-5	7	4	17.8	11.1
5	9	4	69.2	2.1
-5	9	4	187.2	1.5
5	11	4	71.9	3.7
-5	11	4	234.8	1.7
5	13	4	162.8	2.4
-5	13	4	0.0	11.9
5	15	4	124.9	7.6
-5	15	4	40.0	9.9
-5	17	4	44.3	3.7
-5	19	4	32.5	15.4
6	0	4	217.6	2.4
-6	0	4	60.6	2.9
6	2	4	61.9	2.9
-6	2	4	103.5	2.7
6	4	4	5.9	14.3
-6	4	4	307.0	3.1
6	6	4	5.6	14.5
-6	6	4	44.8	4.9
6	8	4	213.8	1.8
-6	8	4	195.1	6.7
6	10	4	78.2	10.8
-6	10	4	27.6	7.2
6	12	4	198.5	9.3
-6	12	4	71.5	6.7
6	14	4	3.8	13.9
-6	14	4	37.5	11.7
-6	16	4	51.5	5.7
-6	18	4	73.4	6.5
7	1	4	89.1	4.0
-7	1	4	349.6	3.7
7	3	4	59.8	2.8
-7	3	4	166.4	3.2
7	5	4	116.0	3.0
-7	5	4	109.3	5.0
7	7	4	11.9	20.0
-7	7	4	135.9	1.9
7	9	4	82.3	4.5
-7	9	4	128.9	4.4
7	11	4	119.8	3.6
-7	11	4	319.3	5.1
7	13	4	16.2	15.6
-7	13	4	27.2	11.5
-7	15	4	8.9	18.1
-7	17	4	39.1	30.6
-7	19	4	71.2	2.9
8	0	4	36.4	6.5
-8	0	4	553.5	2.1
8	2	4	69.6	2.3
-8	2	4	56.9	2.3
8	4	4	106.5	8.8
-8	4	4	22.4	11.6
8	6	4	18.1	20.8
-8	6	4	38.2	5.9
8	8	4	161.1	3.0
-8	8	4	252.8	4.7
8	10	4	19.3	20.9
-8	10	4	139.9	2.0
-8	12	4	421.9	4.6
-8	14	4	11.1	19.4
-8	16	4	178.6	1.9
9	1	4	67.5	4.7
-9	1	4	41.1	6.3
9	3	4	0.0	10.1
-9	3	4	136.9	2.3
9	5	4	54.2	4.4
-9	5	4	10.4	18.6
-9	7	4	128.9	2.6
-9	9	4	32.1	21.1

## fluoro-tremolite 1082\_751\_361.cif

-9	11	4	119.2	5.3
-9	13	4	52.1	5.3
-9	15	4	111.6	2.8
-10	0	4	112.9	2.6
-10	2	4	28.2	13.2
-10	4	4	22.0	12.1
-10	6	4	48.5	14.3
-10	8	4	99.6	5.8
-10	10	4	76.4	2.3
-10	12	4	127.1	5.0
-10	14	4	86.4	4.1
-11	1	4	101.6	3.8
-11	3	4	31.9	5.9
-11	5	4	37.7	3.7
-11	7	4	51.7	3.2
-11	9	4	199.3	2.2
-11	11	4	287.0	2.0
-12	0	4	138.8	2.8
-12	2	4	34.3	6.2
-12	4	4	66.2	3.4
-12	6	4	59.0	7.3
-12	8	4	55.0	3.2
-13	1	4	110.7	6.7
0	0	5	54.0	3.2
0	2	5	161.8	1.6
0	4	5	17.0	14.2
0	6	5	276.5	2.1
0	8	5	46.4	7.8
0	10	5	126.0	4.7
0	12	5	41.1	8.0
0	14	5	317.7	4.4
0	16	5	162.5	8.0
0	18	5	130.9	7.3
1	1	5	10.5	18.5
-1	1	5	51.5	3.4
1	3	5	33.3	12.8
-1	3	5	14.5	12.9
1	5	5	119.9	2.2
-1	5	5	69.2	2.2
1	7	5	23.8	14.6
-1	7	5	109.9	7.5
1	9	5	70.6	2.1
-1	9	5	80.4	5.9
1	11	5	86.1	9.0
-1	11	5	28.3	10.3
1	13	5	53.4	7.4
-1	13	5	108.2	4.3
1	15	5	34.6	6.7
-1	15	5	37.8	4.7
1	17	5	40.8	22.9
-1	17	5	28.4	11.8
2	0	5	40.8	5.4
-2	0	5	65.1	3.2
2	2	5	184.9	1.9
-2	2	5	218.3	2.5
2	4	5	24.3	8.3
-2	4	5	56.0	3.0
2	6	5	23.6	5.8
-2	6	5	167.9	1.7
2	8	5	33.5	4.7
-2	8	5	17.1	13.2
2	10	5	75.5	6.8
-2	10	5	66.5	4.2
2	12	5	77.6	2.6
-2	12	5	34.2	7.4
2	14	5	73.2	2.9
-2	14	5	85.6	8.8
2	16	5	61.3	3.6
-2	16	5	79.3	3.7
-2	18	5	251.4	2.7
3	1	5	19.1	20.4
-3	1	5	53.0	2.8
3	3	5	202.7	2.9
-3	3	5	171.2	5.5
3	5	5	334.3	1.7
-3	5	5	324.0	1.5
3	7	5	120.2	4.6
-3	7	5	67.4	2.0
3	9	5	68.7	6.2
-3	9	5	9.2	10.3
3	11	5	0.0	12.9
-3	11	5	59.4	2.3
3	13	5	46.9	3.5
-3	13	5	63.5	2.5
3	15	5	149.0	10.3
-3	15	5	125.3	10.2
-3	17	5	266.8	2.0
4	0	5	80.7	2.9
-4	0	5	79.8	2.8
4	2	5	16.9	20.1
-4	2	5	0.0	11.6
4	4	5	0.0	12.4
-4	4	5	0.0	10.4
4	6	5	462.7	1.7
-4	6	5	566.3	4.9
4	8	5	14.4	20.2

## fluoro-tremolite 1082\_751\_361.cif

-4	8	5	73.1	6.8
4	10	5	73.7	4.0
-4	10	5	62.9	3.2
4	12	5	18.6	20.8
-4	12	5	50.4	2.6
4	14	5	80.9	2.4
-4	14	5	90.5	2.4
-4	16	5	153.2	1.9
-4	18	5	176.6	5.3
5	1	5	41.4	3.6
-5	1	5	99.2	2.5
5	3	5	106.0	2.0
-5	3	5	32.9	8.2
5	5	5	57.0	7.0
-5	5	5	100.0	1.8
5	7	5	71.4	4.7
-5	7	5	61.7	2.7
5	9	5	146.8	2.3
-5	9	5	159.4	2.2
5	11	5	2.4	13.5
-5	11	5	29.2	12.5
-5	13	5	119.2	2.0
-5	15	5	57.9	3.7
-5	17	5	31.7	8.8
6	0	5	0.0	18.2
-6	0	5	59.0	3.7
6	2	5	48.6	3.2
-6	2	5	64.8	2.3
6	4	5	8.8	17.8
-6	4	5	0.0	11.8
6	6	5	14.7	15.7
-6	6	5	201.3	2.0
6	8	5	5.3	14.8
-6	8	5	20.2	11.4
6	10	5	26.9	5.8
-6	10	5	8.2	13.1
-6	12	5	62.0	2.8
-6	14	5	121.1	2.2
-6	16	5	145.0	6.5
7	1	5	20.1	19.3
-7	1	5	19.8	17.2
7	3	5	111.5	2.5
-7	3	5	189.2	1.9
7	5	5	227.8	3.3
-7	5	5	456.7	4.0
-7	7	5	222.8	1.7
-7	9	5	85.5	2.8
-7	11	5	70.1	2.2
-7	13	5	27.4	5.9
-7	15	5	72.6	5.4
-8	0	5	35.1	4.5
-8	2	5	71.4	6.6
-8	4	5	0.0	12.3
-8	6	5	17.3	14.3
-8	8	5	39.2	4.3
-8	10	5	8.3	16.9
-8	12	5	48.2	3.3
-8	14	5	59.2	9.0
-9	1	5	45.5	7.2
-9	3	5	62.0	2.7
-9	5	5	97.9	2.5
-9	7	5	232.2	5.0
-9	9	5	166.6	2.0
-9	11	5	27.6	10.5
-9	13	5	73.5	3.2
-10	0	5	46.4	4.2
-10	2	5	21.0	22.3
-10	4	5	37.4	12.0
-10	6	5	244.3	3.1
-10	8	5	55.5	3.2
-10	10	5	61.1	5.8
-11	1	5	40.7	13.9
-11	3	5	117.7	4.8
-11	5	5	168.6	2.0
-11	7	5	15.8	15.9
-12	0	5	102.3	3.2
-12	2	5	148.3	5.2
0	0	6	149.4	2.5
0	2	6	66.4	2.9
0	4	6	87.0	2.7
0	6	6	0.0	12.8
0	8	6	106.9	5.0
0	10	6	54.6	4.2
0	12	6	133.9	4.5
0	14	6	20.8	22.7
1	1	6	209.4	1.8
-1	1	6	69.1	3.7
1	3	6	105.0	2.2
-1	3	6	114.8	2.9
1	5	6	109.0	5.0
-1	5	6	30.4	9.7
1	7	6	40.3	4.5
-1	7	6	119.2	9.3
1	9	6	78.0	3.3
-1	9	6	43.9	5.8
1	11	6	196.6	11.4

## fluoro-tremolite 1082\_751\_361.cif

-1	11	6	0.0	13.2
1	13	6	29.0	24.5
-1	13	6	132.3	8.7
2	0	6	142.4	2.7
-2	0	6	476.2	2.3
2	2	6	13.3	17.6
-2	2	6	51.4	7.0
2	4	6	72.8	5.5
-2	4	6	9.6	18.1
2	6	6	44.0	5.2
-2	6	6	36.9	6.6
2	8	6	49.2	3.9
-2	8	6	48.8	3.1
2	10	6	45.5	8.0
-2	10	6	78.2	5.8
-2	12	6	193.9	5.5
-2	14	6	33.2	5.2
3	1	6	113.7	2.1
-3	1	6	277.2	1.7
3	3	6	82.8	7.1
-3	3	6	83.3	3.2
3	5	6	54.6	3.6
-3	5	6	11.6	21.0
3	7	6	56.5	5.9
-3	7	6	52.2	5.5
3	9	6	62.6	6.1
-3	9	6	246.6	2.1
-3	11	6	469.6	5.6
-3	13	6	167.9	2.0
4	0	6	450.5	2.6
-4	0	6	163.2	2.6
4	2	6	67.2	2.8
-4	2	6	50.3	5.3
4	4	6	119.2	3.3
-4	4	6	39.2	7.1
4	6	6	5.3	15.2
-4	6	6	5.5	12.0
-4	8	6	64.6	2.7
-4	10	6	56.7	2.9
-4	12	6	52.7	3.4
-4	14	6	47.0	29.7
5	1	6	93.4	3.1
-5	1	6	11.3	20.3
-5	3	6	84.8	2.7
-5	5	6	25.9	15.2
-5	7	6	149.6	3.0
-5	9	6	34.6	3.7
-5	11	6	34.9	10.8
-5	13	6	79.2	4.6
-6	0	6	227.0	2.5
-6	2	6	44.4	7.6
-6	4	6	18.2	12.7
-6	6	6	30.8	11.8
-6	8	6	220.3	3.2
-6	10	6	99.7	4.2
-6	12	6	193.9	4.3
-7	1	6	61.2	2.8
-7	3	6	45.9	8.7
-7	5	6	111.3	2.2
-7	7	6	65.5	3.3
-7	9	6	63.7	4.9
-7	11	6	89.1	2.7
-8	0	6	83.1	3.3
-8	2	6	71.6	4.5
-8	4	6	169.7	2.6
-8	6	6	11.4	20.8
-8	8	6	167.3	3.9
-8	10	6	46.1	19.5
-9	1	6	26.0	13.6
-9	3	6	0.0	13.2
-9	5	6	3.6	14.3
-9	7	6	19.4	22.3
-9	9	6	149.8	2.4
-10	0	6	473.4	2.7
-10	2	6	90.4	2.9
-10	4	6	91.0	2.6
-10	6	6	47.9	11.1
0	0	7	19.7	18.7
0	2	7	153.1	2.5
0	4	7	44.7	4.3
1	1	7	0.0	13.7
-1	1	7	0.0	13.5
-1	3	7	5.0	14.9
-1	5	7	133.9	3.8
-1	7	7	29.0	9.1
-2	0	7	29.8	6.8
-2	2	7	108.8	7.7
-2	4	7	14.7	14.4
-2	6	7	371.1	2.1
-2	8	7	37.3	12.1
-3	1	7	53.8	5.9
-3	3	7	39.4	7.4
-3	5	7	92.2	6.4
-3	7	7	33.5	6.0
-4	0	7	66.4	4.5
-4	2	7	130.5	2.5

fluoro-tremolite 1082\_751\_361.cif

```

-4  4   7    29.3   11.2
-4  6   7   199.6    8.3
-4  8   7    12.3   17.0
-5  1   7   26.0   11.5
-5  3   7   101.4    2.9
-5  5   7   143.5    3.5
-5  7   7   19.3   20.1
-6  0   7   68.6    4.5
-6  2   7    6.1   16.5
-6  4   7   40.2   32.2
-6  6   7   229.6    4.0
-7  1   7   35.8   10.8
-7  3   7   27.8    8.3

#====END

data_361_AZB

_publ_contact_author
;
Roberta Oberti
;
_publ_contact_author_email
;
oberti@crystal.unipv.it
;

loop_
_publ_author_name
_publ_author_address
'Oberti R.'
'CNR-IGG, S.S. Pavia, Pavia, Italy'
'Camara F.'
'Dip.to di Scienze della Terra, Università di Milano, Milan, Italy'
'Bellatrecchia F.'
'Dip.to di Scienze, Università Roma Tre, Rome, Italy'
'Radica F.'
'Dip.to di Scienze, Università Roma Tre, Rome, Italy'
'Gianfagna A.'
'Dip.to di Scienze della Terra, Università di Roma La Sapienza, Rome, Italy'
'Boiocchi M.'
'Centro Grandi Strumenti, Università di Pavia, Pavia, Italy'

_publ_section_title
;
Fluoro-tremolite from the Limecrest-Southdown quarry, Sparta, NJ, USA:
crystal structure and crystal chemistry of a newly approved end-members
of the amphibole supergroup and its solid solution with tremolite
;

_audit_creation_method      'manually entered'
_chemical_name_systematic   ?
_chemical_name_mineral
;
tremolite
;
_chemical_compound_source
;
Val Tremola, Switzerland
;
_chemical_name_common        ?
_chemical_melting_point     ?
_chemical_formula_moiety    ?
_chemical_formula_sum
'Ca1.99 Fe0 H2 Mg5 Na0.01 O24 Si8'
_chemical_formula_weight     812.24

loop_
_atom_type_symbol
_atom_type_description
_atom_type_scat_dispersion_real
_atom_type_scat_dispersion_imag
_atom_type_scat_source
'O' 'O'  0.0106  0.0060
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'O2-' 'O2-' 0.0106  0.0060
'Hovesteydt, 1982'
'Si' 'Si'  0.0817  0.0784
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Si4+' 'Si4+' 0.0817  0.0710
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Fe2+' 'Fe2+' 0.3460  0.8450
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Mg2+' 'Mg2+' 0.0490  0.0360
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Na+' 'Na+' 0.0360  0.0250
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'Ca2+' 'Ca2+' 0.2260  0.3060
'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'

_space_group_crystal_system      monoclinic
_space_group_IT_number          12
_space_group_name_H-M_alt        'C 2/m'

```

fluoro-tremolite 1082\_751\_361.cif

```

_space_group_name_Hall      '-C 2y'

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

  _cell_length_a            9.8359(3)
  _cell_length_b            18.0450(6)
  _cell_length_c            5.2752(2)
  _cell_angle_alpha          90
  _cell_angle_beta          104.750(3)
  _cell_angle_gamma          90
  _cell_volume              905.44(5)
  _cell_formula_units_Z      2
  _cell_measurement_temperature 298(2)
  _cell_measurement_reflns_used 60
  _cell_measurement_theta_min 2
  _cell_measurement_theta_max 30

  _exptl_crystal_description      'prism'
  _exptl_crystal_colour          'colourless'
  _exptl_crystal_density_meas     ?
  _exptl_crystal_density_method   ?
  _exptl_crystal_density_diffrn  2.980
  _exptl_crystal_F_000           811.9
  _exptl_crystal_size_max        0.330
  _exptl_crystal_size_mid        0.160
  _exptl_crystal_size_min        0.080
  _exptl_absorpt_coefficient_mu  1.470
  _exptl_absorpt_correction_type  psi-scan
  _exptl_absorpt_correction_T_min 0.808
  _exptl_absorpt_correction_T_max 0.931
  _exptl_absorpt_process_details ;
; North A.C.T., Phillips D.C. & Mathews F.S. (1968) Acta. Cryst. A24, 351
; _exptl_absorpt_special_details    ?

  _diffrn_ambient_temperature    298(2)
  _diffrn_radiation_wavelength   0.7107
  _diffrn_radiation_type         MoK\alpha
  _diffrn_radiation_source       'fine-focus sealed tube'
  _diffrn_radiation_monochromator graphite
  _diffrn_measurement_device_type 'PHILIPS PW1100'
  _diffrn_measurement_method     'omega-2theta scans'
  _diffrn_standards_number       3
  _diffrn_standards_interval_count 400
  _diffrn_standards_decay_%      0
  _diffrn_reflns_number          2690
  _diffrn_reflns_av_R_equivalents 0.014
  _diffrn_reflns_limit_h_min     -13
  _diffrn_reflns_limit_h_max     13
  _diffrn_reflns_limit_k_min     -25
  _diffrn_reflns_limit_k_max     25
  _diffrn_reflns_limit_l_min     0
  _diffrn_reflns_limit_l_max     7
  _diffrn_reflns_theta_min       2.257
  _diffrn_reflns_theta_max       29.974
  _diffrn_measured_fraction_theta_max 1.000
  _reflns_number_total          1367
  _reflns_number_gt              1263
  _reflns_threshold_expression   'I > 3\s(I)'

  _reflns_special_details       ?

  _computing_data_collection    'local program'
  _computing_cell_refinement    'LAT routine of PW1100 diffractometer'
  _computing_data_reduction     'local program'
  _computing_structure_refinement 'ORFLS (Busing et al., 1962), modified'

  _refine_special_details       ;
; Refinement of F against reflections with F > 3sigma(F).
; The threshold expression (_gt) of F > 3sigma(F) corresponds to the cutoff used
; to discriminate between observed and unobserved reflections for refinement.
; The use of unitary weight produces unusual values for the calculated
; weighted wR-factor (similar to R).
;

  _refine_ls_structure_factor_coef  F
  _refine_ls_matrix_type          full
  _refine_ls_weighting_scheme     unit
  _refine_ls_hydrogen_treatment   mixed
  _refine_ls_extinction_method    'secondary isotropic'
  _refine_ls_extinction_coef      0.000182(2)
  _refine_ls_extinction_expression 'Zachariasen, 1967'
  _refine_ls_number_reflns        1263
  _refine_ls_number_parameters    113

```

```

fluoro-tremolite 1082_751_361.cif
_refine_ls_R_factor_all      0.0197
_refine_ls_R_factor_gt       0.0174
_refine_ls_wR_factor_ref     0.0239
_refine_ls_wR_factor_gt      0.0223
_refine_ls_restrained_S_all  1.06

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
O1A O 0.11168(10) 0.08595(6) 0.2176(2) 0.0058(3) Uani 0.26(9) 1 d . . P .
O1B O2- 0.11168(10) 0.08595(6) 0.2176(2) 0.0058(3) Uani 0.74(9) 1 d . . P .
O2A O 0.11855(10) 0.17106(6) 0.7242(2) 0.0063(3) Uani 0.27(9) 1 d . . P .
O2B O2- 0.11855(10) 0.17106(6) 0.7242(2) 0.0063(3) Uani 0.73(9) 1 d . . P .
O3A O 0.1097(2) 0.0000 0.7155(3) 0.0070(4) Uani 0.48(6) 2 d S T P .
O3B O2- 0.1097(2) 0.0000 0.7155(3) 0.0070(4) Uani 0.52(6) 2 d S T P .
O4A O 0.36527(11) 0.24795(6) 0.7931(2) 0.0078(3) Uani 0.27(9) 1 d . . P .
O4B O2- 0.36527(11) 0.24795(6) 0.7931(2) 0.0078(3) Uani 0.73(9) 1 d . . P .
O5A O 0.34630(11) 0.13424(6) 0.1000(2) 0.0072(3) Uani 0.37(10) 1 d . . P .
O5B O2- 0.34630(11) 0.13424(6) 0.1000(2) 0.0072(3) Uani 0.63(10) 1 d . . P .
O6A O 0.34370(11) 0.11863(6) 0.5892(2) 0.0073(3) Uani 0.38(10) 1 d . . P .
O6B O2- 0.34370(11) 0.11863(6) 0.5892(2) 0.0073(3) Uani 0.62(10) 1 d . . P .
O7A O 0.3372(2) 0.0000 0.2922(3) 0.0083(4) Uani 0.48(7) 2 d S T P .
O7B O2- 0.3372(2) 0.0000 0.2922(3) 0.0083(4) Uani 0.52(7) 2 d S T P .
T1A Si 0.28025(4) 0.08401(2) 0.29701(8) 0.0042(2) Uani 0.66(7) 1 d . . P .
T1B Si4+ 0.28025(4) 0.08401(2) 0.29701(8) 0.0042(2) Uani 0.34(7) 1 d . . P .
T2A Si 0.28829(4) 0.17113(2) 0.80461(8) 0.0044(2) Uani 0.68(7) 1 d . . P .
T2B Si4+ 0.28829(4) 0.17113(2) 0.80461(8) 0.0044(2) Uani 0.32(7) 1 d . . P .
M1A Mg2+ 0.0000 0.00773(4) 0.5000 0.0052(2) Uani 1.000(3) 2 d S T P .
M1B Fe2+ 0.0000 0.00773(4) 0.5000 0.0052(2) Uani 0.000(3) 2 d S T P .
M2A Mg2+ 0.0000 0.17654(4) 0.0000 0.0050(2) Uani 1.000(3) 2 d S T P .
M2B Fe2+ 0.0000 0.17654(4) 0.0000 0.0050(2) Uani 0.000(3) 2 d S T P .
M3A Mg2+ 0.0000 0.0000 0.0000 0.0049(3) Uani 1.000(3) 4 d S T P .
M3B Fe2+ 0.0000 0.0000 0.0000 0.0049(3) Uani 0.000(3) 4 d S T P .
M4A Ca2+ 0.0000 0.27788(2) 0.5000 0.0077(2) Uani 0.996(7) 2 d S T P .
M4B Na+ 0.0000 0.27788(2) 0.5000 0.0077(2) Uani 0.004(7) 2 d S T P .
H H 0.190(5) 0.0000 0.780(9) 0.050(13) Uiso 1 2 d S . P .

loop_
_atom_site_aniso_label
_atom_site_aniso_U_11
_atom_site_aniso_U_22
_atom_site_aniso_U_33
_atom_site_aniso_U_12
_atom_site_aniso_U_13
_atom_site_aniso_U_23
O1A 0.0047(4) 0.0059(5) 0.0067(4) -0.0002(3) 0.0012(3) -0.0002(4)
O1B 0.0047(4) 0.0059(5) 0.0067(4) -0.0002(3) 0.0012(3) -0.0002(4)
O2A 0.0050(4) 0.0068(5) 0.0072(4) 0.0000(3) 0.0014(3) -0.0004(4)
O2B 0.0050(4) 0.0068(5) 0.0072(4) 0.0000(3) 0.0014(3) -0.0004(4)
O3A 0.0064(6) 0.0066(7) 0.0078(7) 0.0000 0.0015(5) 0.0000
O3B 0.0064(6) 0.0066(7) 0.0078(7) 0.0000 0.0015(5) 0.0000
O4A 0.0088(5) 0.0059(5) 0.0091(5) -0.0019(3) 0.0030(4) -0.0006(4)
O4B 0.0088(5) 0.0059(5) 0.0091(5) -0.0019(3) 0.0030(4) -0.0006(4)
O5A 0.0058(4) 0.0092(5) 0.0064(4) -0.0010(3) 0.0011(3) 0.0023(4)
O5B 0.0058(4) 0.0092(5) 0.0064(4) -0.0010(3) 0.0011(3) 0.0023(4)
O6A 0.0064(4) 0.0094(5) 0.0058(4) 0.0000(3) 0.0012(3) -0.0026(4)
O6B 0.0064(4) 0.0094(5) 0.0058(4) 0.0000(3) 0.0012(3) -0.0026(4)
O7A 0.0074(6) 0.0041(7) 0.0131(7) 0.0000 0.0022(5) 0.0000
O7B 0.0074(6) 0.0041(7) 0.0131(7) 0.0000 0.0022(5) 0.0000
T1A 0.00417(14) 0.0040(2) 0.0043(2) -0.00044(9) 0.00062(12) -0.00023(14)
T1B 0.00417(14) 0.0040(2) 0.0043(2) -0.00044(9) 0.00062(12) -0.00023(14)
T2A 0.00417(14) 0.0046(2) 0.0041(2) -0.00070(9) 0.00074(12) -0.00019(14)
T2B 0.00417(14) 0.0046(2) 0.0041(2) -0.00070(9) 0.00074(12) -0.00019(14)
M1A 0.0057(4) 0.0046(3) 0.0053(4) 0.0000 0.0016(2) 0.0000
M1B 0.0057(4) 0.0046(3) 0.0053(4) 0.0000 0.0016(2) 0.0000
M2A 0.0051(4) 0.0045(3) 0.0056(4) 0.0000 0.0015(2) 0.0000
M2B 0.0051(4) 0.0045(3) 0.0056(4) 0.0000 0.0015(2) 0.0000
M3A 0.0050(5) 0.0046(5) 0.0050(5) 0.0000 0.0009(3) 0.0000
M3B 0.0050(5) 0.0046(5) 0.0050(5) 0.0000 0.0009(3) 0.0000
M4A 0.0092(2) 0.0063(2) 0.0094(2) 0.0000 0.0055(2) 0.0000
M4B 0.0092(2) 0.0063(2) 0.0094(2) 0.0000 0.0055(2) 0.0000

_geom_special_details
;
Geometry data (distances and angles) are reported only for T and M
sites flagged by the A suffix.
All esds are estimated using the full covariance matrix.
;

loop_
_geom_bond_atom_site_label_1
_geom_bond_atom_site_label_2
_geom_bond_distance

```

fluoro-tremolite 1082\_751\_361.cif

```

_geom_bond_site_symmetry_2
_geom_bond_publ_flag
T1A O1A 1.6038(11) . ?
T1A O7A 1.6184(7) . ?
T1A O6A 1.6327(11) . ?
T1A O5A 1.6334(11) . ?
T2A O4A 1.5881(11) . ?
T2A O2A 1.6145(11) . ?
T2A O5A 1.6564(11) 1_556 ?
T2A O6A 1.6737(11) . ?
M1A O1A 2.0640(10) 6_556 ?
M1A O1A 2.0640(10) . ?
M1A O2A 2.0777(11) 6_556 ?
M1A O2A 2.0777(11) . ?
M1A O3A 2.0828(10) 5_556 ?
M1A O3A 2.0828(10) . ?
M2A O4A 2.0168(11) 7_556 ?
M2A O4A 2.0168(11) 4_454 ?
M2A O2A 2.0859(10) 6_556 ?
M2A O2A 2.0859(10) 1_554 ?
M2A O1A 2.1341(12) 6 ?
M2A O1A 2.1341(12) . ?
M3A O3A 2.059(2) 5_556 ?
M3A O3A 2.059(2) 1_554 ?
M3A O1A 2.0707(10) . ?
M3A O1A 2.0707(10) 5 ?
M3A O1A 2.0707(10) 2 ?
M3A O1A 2.0707(10) 6 ?
M4A O4A 2.3253(10) 4_455 ?
M4A O4A 2.3253(10) 7_556 ?
M4A O2A 2.4924(11) . ?
M4A O2A 2.4924(11) 6_556 ?
M4A O6A 2.5379(11) 7_556 ?
M4A O6A 2.5379(11) 4_455 ?
M4A O5A 2.7621(11) 7_556 ?
M4A O5A 2.7621(11) 4_455 ?
O3A H 0.77(5) . ?

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
O1A T1A O7A 110.80(6) . . ?
O1A T1A O6A 111.07(6) . . ?
O7A T1A O6A 108.82(7) . . ?
O1A T1A O5A 111.96(6) . . ?
O7A T1A O5A 108.33(7) . . ?
O6A T1A O5A 105.67(6) . . ?
O4A T2A O2A 117.50(6) . . ?
O4A T2A O5A 109.48(6) 1_556 ?
O2A T2A O5A 109.42(5) 1_556 ?
O4A T2A O6A 103.14(6) . . ?
O2A T2A O6A 108.35(6) . . ?
O5A T2A O6A 108.51(6) 1_556 . ?
O1A M1A O1A 178.22(10) 6_556 . ?
O1A M1A O2A 95.58(4) 6_556 6_556 ?
O1A M1A O2A 85.71(4) . 6_556 ?
O1A M1A O2A 85.71(4) 6_556 . ?
O1A M1A O2A 95.58(4) . . ?
O2A M1A O2A 87.28(6) 6_556 . ?
O1A M1A O3A 94.89(5) 6_556 5_556 ?
O1A M1A O3A 83.75(5) . 5_556 ?
O2A M1A O3A 95.84(4) 6_556 5_556 ?
O2A M1A O3A 176.75(5) . 5_556 ?
O1A M1A O3A 83.75(5) 6_556 . ?
O1A M1A O3A 94.89(5) . . ?
O2A M1A O3A 176.75(5) 6_556 . ?
O2A M1A O3A 95.84(4) . . ?
O3A M1A O3A 81.06(7) 5_556 . ?
O4A M2A O4A 94.99(7) 7_556 4_454 ?
O4A M2A O2A 93.53(4) 7_556 6_556 ?
O4A M2A O2A 90.15(4) 4_454 6_556 ?
O4A M2A O2A 90.15(4) 7_556 1_554 ?
O4A M2A O2A 93.53(4) 4_454 1_554 ?
O2A M2A O2A 174.56(7) 6_556 1_554 ?
O4A M2A O1A 170.37(5) 7_556 6 ?
O4A M2A O1A 92.81(4) 4_454 6 ?
O2A M2A O1A 92.08(4) 6_556 6 ?
O2A M2A O1A 83.74(4) 1_554 6 ?
O4A M2A O1A 92.81(4) 7_556 . ?
O4A M2A O1A 170.37(5) 4_454 . ?
O2A M2A O1A 83.74(4) 6_556 . ?
O2A M2A O1A 92.08(4) 1_554 . ?
O1A M2A O1A 80.01(6) 6 . ?
O3A M3A O3A 180.0 5_556 1_554 ?
O3A M3A O1A 84.17(4) 5_556 . ?
O3A M3A O1A 95.83(4) 1_554 . ?
O3A M3A O1A 95.83(4) 5_556 5 ?
O3A M3A O1A 84.17(4) 1_554 5 ?
O1A M3A O1A 180.0 . 5 ?
O3A M3A O1A 84.17(4) 5_556 2 ?
O3A M3A O1A 95.83(4) 1_554 2 ?

```

## fluoro-tremolite 1082\_751\_361.cif

01A M3A 01A 97.01(6) . 2 ?  
 01A M3A 01A 82.99(6) 5 2 ?  
 03A M3A 01A 95.83(4) 5\_556 6 ?  
 03A M3A 01A 84.17(4) 1\_554 6 ?  
 01A M3A 01A 82.99(6) . 6 ?  
 01A M3A 01A 97.01(6) 5 6 ?  
 01A M3A 01A 180.0 2 6 ?  
 04A M4A 04A 156.88(6) 4\_455 7\_556 ?  
 04A M4A 02A 78.42(4) 4\_455 . ?  
 04A M4A 02A 83.06(4) 7\_556 . ?  
 04A M4A 02A 83.06(4) 4\_455 6\_556 ?  
 04A M4A 02A 78.42(4) 7\_556 6\_556 ?  
 02A M4A 02A 73.29(5) . 6\_556 ?  
 04A M4A 06A 138.20(4) 4\_455 7\_556 ?  
 04A M4A 06A 63.23(4) 7\_556 7\_556 ?  
 02A M4A 06A 116.15(3) . 7\_556 ?  
 02A M4A 06A 137.75(3) 6\_556 7\_556 ?  
 04A M4A 06A 63.23(4) 4\_455 4\_455 ?  
 04A M4A 06A 138.20(4) 7\_556 4\_455 ?  
 02A M4A 06A 137.75(3) . 4\_455 ?  
 02A M4A 06A 116.15(3) 6\_556 4\_455 ?  
 06A M4A 06A 85.24(5) 7\_556 4\_455 ?  
 04A M4A 05A 84.31(3) 4\_455 7\_556 ?  
 04A M4A 05A 109.23(3) 7\_556 7\_556 ?  
 02A M4A 05A 88.97(3) . 7\_556 ?  
 02A M4A 05A 159.95(4) 6\_556 7\_556 ?  
 06A M4A 05A 58.64(3) 7\_556 7\_556 ?  
 06A M4A 05A 71.06(3) 4\_455 7\_556 ?  
 04A M4A 05A 109.23(3) 4\_455 4\_455 ?  
 04A M4A 05A 84.31(3) 7\_556 4\_455 ?  
 02A M4A 05A 159.95(4) . 4\_455 ?  
 02A M4A 05A 88.97(3) 6\_556 4\_455 ?  
 06A M4A 05A 71.06(3) 7\_556 4\_455 ?  
 06A M4A 05A 58.64(3) 4\_455 4\_455 ?  
 05A M4A 05A 109.92(5) 7\_556 4\_455 ?  
 T1A 05A T2A 136.39(7) . 1\_554 ?  
 T1A 06A T2A 138.19(7) . . ?  
 T1A 07A T1A 139.00(10) 2 . ?  
 05A 06A 05A 167.76(6) . 1\_556 ?  
 06A 07A 06A 108.13(7) . 2 ?

\_refine\_diff\_density\_max 0.37  
 \_refine\_diff\_density\_min -0.35

loop\_  
 \_refln\_index\_h  
 \_refln\_index\_k  
 \_refln\_index\_l  
 \_refln\_F\_meas  
 \_refln\_F\_sigma

0	2	0	260.1	1.2
0	4	0	376.1	1.6
0	6	0	37.5	0.6
0	8	0	103.2	0.6
0	10	0	314.2	0.8
0	12	0	833.8	3.2
0	14	0	21.3	1.2
0	16	0	51.5	1.0
0	18	0	86.1	1.0
0	20	0	359.3	1.2
0	22	0	359.3	1.2
0	24	0	466.4	1.2
1	1	0	246.7	0.8
1	3	0	184.6	0.4
1	5	0	20.5	1.3
1	7	0	35.7	0.6
1	9	0	335.8	2.0
1	11	0	615.1	4.0
1	13	0	47.8	1.6
1	15	0	32.4	2.5
1	17	0	29.5	3.7
1	19	0	25.2	5.1
1	21	0	123.3	1.0
1	23	0	62.0	2.4
1	25	0	70.8	2.1
2	0	0	184.3	0.4
2	2	0	186.0	1.6
2	4	0	466.9	1.6
2	6	0	65.7	0.4
2	8	0	74.8	0.9
2	10	0	127.3	0.5
2	12	0	225.5	1.0
2	14	0	138.0	0.8
2	16	0	58.3	0.8
2	18	0	151.6	0.8
2	20	0	66.7	2.8
2	22	0	101.8	2.1
2	24	0	210.0	3.4
3	1	0	611.5	2.4
3	3	0	282.6	0.4
3	5	0	305.1	3.2
3	7	0	367.8	1.2
3	9	0	95.2	1.8
3	11	0	407.8	1.2

## fluoro-tremolite 1082\_751\_361.cif

3	13	0	11.2	7.4
3	15	0	40.2	1.0
3	17	0	107.9	0.7
3	19	0	164.3	2.6
3	21	0	36.7	1.3
3	23	0	182.3	3.0
4	0	0	31.2	0.7
4	2	0	85.5	0.4
4	4	0	46.6	1.3
4	6	0	73.1	0.7
4	8	0	461.6	0.8
4	10	0	232.5	1.0
4	12	0	208.5	0.8
4	14	0	86.3	1.6
4	16	0	323.8	2.4
4	18	0	99.3	2.2
4	20	0	249.1	3.4
4	22	0	215.1	1.6
4	24	0	3.2	6.2
5	1	0	428.4	2.0
5	3	0	341.8	1.6
5	5	0	74.0	0.7
5	7	0	191.5	0.6
5	9	0	26.4	0.7
5	11	0	136.7	1.6
5	13	0	293.3	3.6
5	15	0	203.6	3.2
5	17	0	19.8	5.4
5	19	0	47.7	2.6
5	21	0	194.4	2.6
5	23	0	285.1	4.0
6	0	0	512.7	0.8
6	2	0	191.9	1.0
6	4	0	55.9	0.7
6	6	0	61.6	1.4
6	8	0	276.8	1.6
6	10	0	57.2	1.0
6	12	0	118.6	1.6
6	14	0	60.2	0.8
6	16	0	76.4	0.8
6	18	0	157.8	0.8
6	20	0	70.3	0.9
6	22	0	111.3	2.0
7	1	0	357.0	0.8
7	3	0	172.4	2.0
7	5	0	55.5	1.9
7	7	0	120.5	1.9
7	9	0	467.0	2.0
7	11	0	691.0	2.4
7	13	0	196.9	1.4
7	15	0	241.9	3.4
7	17	0	39.7	1.0
7	19	0	137.8	3.6
7	21	0	34.4	2.4
8	0	0	520.2	0.8
8	2	0	123.8	1.0
8	4	0	106.5	1.7
8	6	0	146.1	1.0
8	8	0	24.6	1.5
8	10	0	115.8	0.8
8	12	0	208.0	1.2
8	14	0	42.0	2.1
8	16	0	56.7	0.9
8	18	0	13.7	6.3
8	20	0	67.8	2.2
9	1	0	120.4	0.9
9	3	0	102.2	0.7
9	5	0	25.6	1.0
9	7	0	311.0	0.8
9	9	0	86.7	3.2
9	11	0	97.1	1.8
9	13	0	121.0	2.3
9	15	0	183.4	3.8
9	17	0	95.4	0.9
10	0	0	407.4	1.2
10	2	0	70.5	1.3
10	4	0	22.3	2.5
10	6	0	56.3	1.1
10	8	0	290.7	1.2
10	10	0	157.1	3.0
10	12	0	338.8	2.0
10	14	0	12.1	11.4
10	16	0	214.5	2.4
11	1	0	273.1	1.2
11	3	0	71.2	1.0
11	5	0	161.0	3.0
11	7	0	0.0	11.9
11	9	0	120.1	1.0
11	11	0	334.5	2.0
11	13	0	77.9	1.7
12	0	0	51.8	1.4
12	2	0	23.1	1.8
12	4	0	105.4	1.4
12	6	0	35.9	3.0
12	8	0	186.4	4.2
12	10	0	95.2	1.6

## fluoro-tremolite 1082\_751\_361.cif

13	1	0	167.7	1.8
13	3	0	92.2	1.7
13	5	0	56.5	1.3
0	0	1	170.4	0.4
0	2	1	70.3	0.3
0	4	1	58.8	1.2
0	6	1	550.9	2.4
0	8	1	73.4	0.5
0	10	1	257.8	1.6
0	12	1	147.1	2.4
0	14	1	200.3	1.2
0	16	1	282.2	0.8
0	18	1	10.4	5.6
0	20	1	64.1	1.6
0	22	1	28.6	1.8
0	24	1	19.1	1.8
1	1	1	116.1	0.3
-1	1	1	294.6	1.2
1	3	1	516.9	8.0
-1	3	1	333.5	2.0
1	5	1	826.9	11.2
-1	5	1	235.5	2.8
1	7	1	277.2	0.8
-1	7	1	480.8	2.0
1	9	1	120.0	2.5
-1	9	1	496.1	0.8
1	11	1	110.5	0.6
-1	11	1	55.2	0.7
1	13	1	177.3	0.8
-1	13	1	270.5	0.4
1	15	1	299.0	0.8
-1	15	1	207.7	1.0
1	17	1	619.8	0.8
-1	17	1	234.4	2.2
1	19	1	236.6	3.0
-1	19	1	111.1	0.8
1	21	1	296.9	2.4
-1	21	1	115.3	1.1
1	23	1	37.7	3.5
-1	23	1	122.5	1.8
-1	25	1	31.9	1.5
2	0	1	189.3	0.6
-2	0	1	165.3	0.4
2	2	1	540.0	5.6
-2	2	1	25.6	0.6
2	4	1	67.6	0.6
-2	4	1	94.5	1.9
2	6	1	661.8	8.8
-2	6	1	272.8	4.0
2	8	1	17.9	0.9
-2	8	1	11.7	1.1
2	10	1	197.8	0.8
-2	10	1	84.9	0.5
2	12	1	89.5	0.7
-2	12	1	125.4	1.1
2	14	1	121.5	0.6
-2	14	1	352.7	0.8
2	16	1	256.2	0.8
-2	16	1	244.6	2.2
2	18	1	7.1	4.4
-2	18	1	109.9	2.2
2	20	1	93.9	0.9
-2	20	1	82.5	1.1
2	22	1	74.4	2.5
-2	22	1	189.1	1.4
2	24	1	35.6	1.4
-2	24	1	60.9	1.3
3	1	1	121.8	0.6
-3	1	1	123.0	0.3
3	3	1	137.9	0.6
-3	3	1	450.7	2.0
3	5	1	506.4	8.8
-3	5	1	625.3	1.6
3	7	1	8.2	2.0
-3	7	1	167.3	0.4
3	9	1	108.5	1.4
-3	9	1	182.3	2.2
3	11	1	93.1	1.2
-3	11	1	239.5	2.0
3	13	1	223.1	1.0
-3	13	1	14.6	3.1
3	15	1	49.0	1.5
-3	15	1	144.0	0.8
3	17	1	100.9	1.2
-3	17	1	329.0	2.8
3	19	1	33.2	1.2
-3	19	1	86.4	0.8
3	21	1	22.5	1.3
-3	21	1	127.4	1.0
3	23	1	136.9	2.8
-3	23	1	120.5	1.7
4	0	1	161.7	0.8
-4	0	1	186.7	0.6
4	2	1	198.3	1.6
-4	2	1	462.1	1.6
4	4	1	19.5	1.5

## fluoro-tremolite 1082\_751\_361.cif

-4	4	1	82.0	0.4
4	6	1	812.9	8.8
-4	6	1	224.1	1.0
4	8	1	105.8	0.5
-4	8	1	12.7	1.1
4	10	1	159.6	1.0
-4	10	1	179.5	1.0
4	12	1	75.4	1.4
-4	12	1	85.6	1.3
4	14	1	495.9	2.4
-4	14	1	29.6	0.8
4	16	1	346.0	4.4
-4	16	1	210.6	2.4
4	18	1	427.5	3.6
-4	18	1	93.0	0.9
4	20	1	37.0	1.7
-4	20	1	109.2	1.0
4	22	1	207.3	2.4
-4	22	1	19.0	3.3
-4	24	1	40.1	2.3
5	1	1	35.6	1.7
-5	1	1	122.4	0.9
5	3	1	49.8	1.0
-5	3	1	77.5	0.5
5	5	1	439.5	2.8
-5	5	1	193.9	0.6
5	7	1	117.2	1.0
-5	7	1	224.1	0.8
5	9	1	137.3	1.2
-5	9	1	230.5	1.8
5	11	1	140.6	0.8
-5	11	1	30.5	0.9
5	13	1	59.3	0.8
-5	13	1	113.6	1.2
5	15	1	53.8	0.9
-5	15	1	26.4	1.3
5	17	1	202.5	2.0
-5	17	1	83.4	1.9
5	19	1	80.9	2.7
-5	19	1	27.2	1.5
5	21	1	16.3	3.2
-5	21	1	59.8	1.6
-5	23	1	62.0	1.4
6	0	1	83.4	0.8
-6	0	1	135.4	0.8
6	2	1	265.2	1.8
-6	2	1	125.0	1.4
6	4	1	12.3	1.5
-6	4	1	66.5	3.5
6	6	1	406.9	3.6
-6	6	1	1003.0	10.4
6	8	1	68.2	0.9
-6	8	1	166.6	0.8
6	10	1	31.0	3.5
-6	10	1	229.2	0.8
6	12	1	133.3	2.5
-6	12	1	90.7	1.5
6	14	1	96.6	0.8
-6	14	1	252.6	0.8
6	16	1	112.5	0.9
-6	16	1	293.3	1.6
6	18	1	472.5	4.0
-6	18	1	339.7	2.0
6	20	1	185.3	2.0
-6	20	1	41.0	1.0
-6	22	1	18.3	3.8
7	1	1	42.5	2.5
-7	1	1	11.4	1.6
7	3	1	179.2	2.8
-7	3	1	142.0	0.6
7	5	1	144.9	0.8
-7	5	1	628.1	2.4
7	7	1	142.7	1.4
-7	7	1	252.6	1.0
7	9	1	52.0	2.2
-7	9	1	55.0	1.2
7	11	1	10.0	3.2
-7	11	1	74.7	0.9
7	13	1	20.6	1.9
-7	13	1	17.8	4.4
7	15	1	142.3	1.2
-7	15	1	62.5	1.0
7	17	1	128.7	0.8
-7	17	1	433.7	1.6
7	19	1	27.8	2.6
-7	19	1	191.5	1.4
-7	21	1	111.2	1.0
8	0	1	103.4	1.0
-8	0	1	80.4	0.9
8	2	1	56.4	0.7
-8	2	1	220.6	3.0
8	4	1	27.6	2.7
-8	4	1	6.6	6.4
8	6	1	530.8	3.2
-8	6	1	173.6	1.2
8	8	1	38.2	1.3

## fluoro-tremolite 1082\_751\_361.cif

-8	8	1	70.8	0.9
8	10	1	134.6	0.8
-8	10	1	68.3	1.1
8	12	1	36.4	1.4
-8	12	1	85.8	1.0
8	14	1	190.3	1.8
-8	14	1	17.6	2.7
8	16	1	224.2	1.8
-8	16	1	181.5	3.0
8	18	1	139.7	1.8
-8	18	1	242.6	2.2
-8	20	1	133.0	1.2
9	1	1	5.6	4.9
-9	1	1	65.7	1.2
9	3	1	27.1	2.0
-9	3	1	129.8	0.7
9	5	1	68.0	0.9
-9	5	1	248.2	1.2
9	7	1	154.2	2.2
-9	7	1	15.4	2.1
9	9	1	151.1	1.2
-9	9	1	16.7	2.3
9	11	1	106.4	2.1
-9	11	1	64.5	2.2
9	13	1	95.3	1.4
-9	13	1	127.8	2.5
9	15	1	42.1	1.4
-9	15	1	15.4	12.2
9	17	1	37.5	1.2
-9	17	1	46.5	4.2
-9	19	1	27.7	5.3
10	0	1	26.6	1.7
-10	0	1	76.0	1.1
10	2	1	185.6	1.4
-10	2	1	81.3	1.2
10	4	1	133.0	1.1
-10	4	1	47.0	0.8
10	6	1	93.1	0.8
-10	6	1	383.4	1.2
10	8	1	101.0	0.9
-10	8	1	19.3	2.2
10	10	1	112.7	1.7
-10	10	1	104.2	1.5
10	12	1	86.3	0.9
-10	12	1	68.3	1.1
10	14	1	58.8	1.1
-10	14	1	283.0	0.8
-10	16	1	248.9	1.0
11	1	1	30.4	3.6
-11	1	1	19.4	3.5
11	3	1	237.5	1.2
-11	3	1	31.5	1.4
11	5	1	504.0	1.2
-11	5	1	38.2	1.0
11	7	1	249.2	1.2
-11	7	1	198.5	1.8
11	9	1	195.7	1.2
-11	9	1	182.6	3.2
11	11	1	40.9	1.1
-11	11	1	125.7	1.1
-11	13	1	27.9	1.5
-11	15	1	29.7	1.6
12	0	1	142.5	1.4
-12	0	1	55.6	1.3
12	2	1	27.6	3.2
-12	2	1	217.3	1.0
12	4	1	76.4	1.1
-12	4	1	137.9	1.0
12	6	1	284.7	4.8
-12	6	1	50.3	1.6
12	8	1	37.7	2.6
-12	8	1	87.5	0.9
-12	10	1	65.8	1.0
-12	12	1	79.6	3.2
-13	1	1	40.8	3.2
-13	3	1	187.3	2.8
-13	5	1	324.3	3.6
-13	7	1	75.9	1.0
0	0	2	432.8	2.4
0	2	2	157.2	0.6
0	4	2	57.9	0.5
0	6	2	36.3	0.6
0	8	2	196.1	0.6
0	10	2	63.9	1.5
0	12	2	585.6	0.8
0	14	2	162.9	1.6
0	16	2	35.6	0.8
0	18	2	148.1	1.0
0	20	2	26.1	1.8
0	22	2	60.0	1.0
0	24	2	302.2	0.8
1	1	2	27.4	1.7
-1	1	2	36.1	0.4
1	3	2	184.8	1.6
-1	3	2	68.9	0.7
1	5	2	105.2	0.7

## fluoro-tremolite 1082\_751\_361.cif

-1	5	2	238.2	0.8
1	7	2	82.1	1.5
-1	7	2	326.2	0.8
1	9	2	402.8	1.6
-1	9	2	17.8	0.9
1	11	2	589.6	0.8
-1	11	2	58.0	1.6
1	13	2	151.5	1.4
-1	13	2	217.8	0.8
1	15	2	157.5	3.0
-1	15	2	183.7	0.8
1	17	2	13.6	12.5
-1	17	2	31.6	2.8
1	19	2	84.2	0.8
-1	19	2	32.9	1.9
1	21	2	69.2	2.7
-1	21	2	141.7	0.8
1	23	2	103.6	2.4
-1	23	2	94.4	1.0
2	0	2	702.0	2.4
-2	0	2	846.5	2.4
2	2	2	124.8	0.8
-2	2	2	192.8	2.0
2	4	2	263.2	3.0
-2	4	2	350.0	0.4
2	6	2	37.7	0.9
-2	6	2	73.5	0.5
2	8	2	56.5	0.7
-2	8	2	449.3	0.4
2	10	2	186.3	0.8
-2	10	2	267.5	4.0
2	12	2	104.9	0.8
-2	12	2	823.4	11.2
2	14	2	92.1	1.1
-2	14	2	25.5	1.4
2	16	2	124.0	1.2
-2	16	2	259.2	0.8
2	18	2	78.6	0.9
-2	18	2	106.2	2.2
2	20	2	263.5	1.0
-2	20	2	227.9	1.0
2	22	2	223.7	1.4
-2	22	2	286.5	1.6
-2	24	2	287.5	1.6
3	1	2	139.0	2.8
-3	1	2	509.7	4.8
3	3	2	169.4	1.0
-3	3	2	236.6	1.2
3	5	2	121.7	0.7
-3	5	2	292.8	2.0
3	7	2	242.6	0.6
-3	7	2	216.6	1.2
3	9	2	11.4	2.9
-3	9	2	197.3	2.6
3	11	2	4.6	3.8
-3	11	2	455.0	4.4
3	13	2	254.4	0.8
-3	13	2	32.4	1.2
3	15	2	169.7	0.8
-3	15	2	15.6	2.1
3	17	2	18.5	7.0
-3	17	2	19.0	1.3
3	19	2	41.4	3.9
-3	19	2	117.1	1.3
3	21	2	151.3	1.2
-3	21	2	43.9	1.0
3	23	2	172.1	3.8
-3	23	2	142.3	2.0
4	0	2	557.7	0.8
-4	0	2	575.5	2.4
4	2	2	192.7	1.6
-4	2	2	180.1	0.6
4	4	2	406.9	1.6
-4	4	2	284.5	2.0
4	6	2	34.6	0.8
-4	6	2	47.7	0.5
4	8	2	107.6	0.9
-4	8	2	331.6	1.2
4	10	2	131.7	1.5
-4	10	2	109.5	1.0
4	12	2	441.8	0.8
-4	12	2	65.5	1.0
4	14	2	16.8	2.9
-4	14	2	100.4	2.8
4	16	2	81.2	0.9
-4	16	2	71.8	0.7
4	18	2	155.1	1.0
-4	18	2	120.6	1.6
4	20	2	21.5	2.3
-4	20	2	67.9	1.0
4	22	2	169.7	1.2
-4	22	2	127.5	0.8
5	1	2	731.3	2.4
-5	1	2	360.7	2.0
5	3	2	384.4	1.6
-5	3	2	97.8	0.7

## fluoro-tremolite 1082\_751\_361.cif

5	5	2	246.3	3.4
-5	5	2	112.0	0.5
5	7	2	99.4	0.6
-5	7	2	8.4	5.4
5	9	2	290.5	2.0
-5	9	2	354.1	2.8
5	11	2	662.0	0.8
-5	11	2	711.9	0.8
5	13	2	189.7	1.4
-5	13	2	220.6	0.8
5	15	2	114.8	1.7
-5	15	2	138.2	1.0
5	17	2	34.5	2.4
-5	17	2	22.5	2.3
5	19	2	218.7	1.6
-5	19	2	39.2	2.1
5	21	2	38.9	1.4
-5	21	2	83.6	3.0
-5	23	2	200.8	9.8
6	0	2	340.0	0.8
-6	0	2	809.4	3.2
6	2	2	51.3	1.4
-6	2	2	66.2	2.2
6	4	2	106.4	0.8
-6	4	2	371.0	0.8
6	6	2	139.5	0.8
-6	6	2	38.8	1.2
6	8	2	15.9	1.9
-6	8	2	226.3	1.0
6	10	2	160.1	0.8
-6	10	2	236.8	1.4
6	12	2	76.1	1.5
-6	12	2	250.9	1.0
6	14	2	87.7	0.8
-6	14	2	67.7	1.3
6	16	2	88.2	2.2
-6	16	2	204.0	1.2
6	18	2	36.2	1.7
-6	18	2	76.7	0.9
6	20	2	53.7	2.8
-6	20	2	354.2	0.8
-6	22	2	269.8	2.0
7	1	2	137.8	1.2
-7	1	2	158.3	2.4
7	3	2	301.7	1.6
-7	3	2	251.3	0.8
7	5	2	118.0	1.0
-7	5	2	91.7	1.3
7	7	2	159.5	0.8
-7	7	2	203.8	1.2
7	9	2	10.3	7.4
-7	9	2	78.1	3.1
7	11	2	117.8	2.7
-7	11	2	42.0	1.4
7	13	2	76.1	3.2
-7	13	2	203.2	1.0
7	15	2	113.3	1.5
-7	15	2	198.2	3.0
7	17	2	33.3	2.2
-7	17	2	9.1	8.4
7	19	2	108.8	1.8
-7	19	2	27.0	4.2
-7	21	2	191.9	1.2
8	0	2	508.9	1.2
-8	0	2	205.4	1.0
8	2	2	63.1	3.4
-8	2	2	82.6	1.0
8	4	2	220.9	2.6
-8	4	2	341.8	0.4
8	6	2	69.3	2.0
-8	6	2	52.0	1.0
8	8	2	96.4	1.4
-8	8	2	18.1	1.9
8	10	2	130.9	3.1
-8	10	2	83.6	0.7
8	12	2	73.1	1.0
-8	12	2	139.3	3.4
8	14	2	56.8	1.8
-8	14	2	108.3	2.3
8	16	2	101.0	2.2
-8	16	2	86.5	1.2
-8	18	2	179.1	1.0
-8	20	2	30.5	1.6
9	1	2	87.4	1.0
-9	1	2	311.9	0.8
9	3	2	0.0	3.9
-9	3	2	286.8	1.2
9	5	2	144.5	1.6
-9	5	2	228.5	2.6
9	7	2	58.9	2.8
-9	7	2	70.3	1.0
9	9	2	138.8	1.0
-9	9	2	253.4	1.2
9	11	2	236.4	1.6
-9	11	2	317.4	1.2
9	13	2	2.8	7.3

## fluoro-tremolite 1082\_751\_361.cif

-9	13	2	23.1	3.7
9	15	2	32.5	1.4
-9	15	2	75.3	1.2
-9	17	2	18.4	3.8
-9	19	2	190.3	3.4
10	0	2	212.6	1.2
-10	0	2	323.7	1.2
10	2	2	52.0	2.8
-10	2	2	127.0	1.4
10	4	2	286.4	1.6
-10	4	2	125.1	0.8
10	6	2	38.8	3.2
-10	6	2	142.0	1.8
10	8	2	121.8	1.4
-10	8	2	20.3	1.3
10	10	2	27.2	2.1
-10	10	2	59.6	1.2
10	12	2	191.5	5.2
-10	12	2	107.6	1.4
-10	14	2	32.9	1.1
-10	16	2	52.9	1.0
11	1	2	57.5	3.2
-11	1	2	135.8	2.2
11	3	2	99.2	1.8
-11	3	2	230.8	1.0
11	5	2	34.2	3.8
-11	5	2	73.7	1.6
11	7	2	198.1	1.0
-11	7	2	144.0	1.4
11	9	2	81.7	1.0
-11	9	2	36.6	2.7
-11	11	2	101.8	1.8
-11	13	2	99.9	0.9
-11	15	2	97.8	1.0
-12	0	2	548.2	1.6
-12	2	2	142.7	0.8
-12	4	2	123.0	2.7
-12	6	2	42.8	3.1
-12	8	2	41.2	1.6
-12	10	2	55.2	1.0
-12	12	2	159.7	2.6
-13	1	2	304.0	1.2
-13	3	2	69.0	1.2
-13	5	2	85.1	4.2
-13	7	2	23.4	4.5
0	0	3	201.8	0.8
0	2	3	419.4	3.2
0	4	3	23.5	1.0
0	6	3	201.4	1.4
0	8	3	18.2	1.2
0	10	3	202.2	1.2
0	12	3	83.2	0.8
0	14	3	93.4	0.8
0	16	3	182.8	1.8
0	18	3	92.0	1.8
0	20	3	110.9	0.8
0	22	3	22.0	10.8
1	1	3	138.0	0.8
-1	1	3	95.2	0.5
1	3	3	17.5	1.2
-1	3	3	446.2	2.0
1	5	3	152.6	2.6
-1	5	3	791.9	5.6
1	7	3	159.4	1.8
-1	7	3	362.6	1.2
1	9	3	237.9	1.2
-1	9	3	216.0	1.0
1	11	3	17.8	2.3
-1	11	3	211.7	0.8
1	13	3	92.1	0.7
-1	13	3	14.9	2.2
1	15	3	5.2	8.4
-1	15	3	149.5	1.0
1	17	3	96.7	2.3
-1	17	3	455.1	2.8
1	19	3	16.7	5.0
-1	19	3	117.8	4.7
1	21	3	52.5	3.1
-1	21	3	139.8	0.8
-1	23	3	102.7	0.9
2	0	3	114.2	0.8
-2	0	3	104.1	0.7
2	2	3	268.6	1.6
-2	2	3	25.2	1.0
2	4	3	26.7	1.6
-2	4	3	27.6	1.4
2	6	3	496.7	3.6
-2	6	3	819.9	2.4
2	8	3	63.4	1.9
-2	8	3	76.2	1.4
2	10	3	334.9	1.2
-2	10	3	32.0	1.0
2	12	3	78.4	2.3
-2	12	3	82.3	0.6
2	14	3	326.1	0.8
-2	14	3	325.6	1.2

## fluoro-tremolite 1082\_751\_361.cif

2	16	3	257.5	2.8
-2	16	3	328.0	0.8
2	18	3	55.5	1.2
-2	18	3	386.1	0.8
2	20	3	31.8	1.5
-2	20	3	18.3	1.8
2	22	3	85.2	2.3
-2	22	3	117.7	1.3
3	1	3	12.2	3.4
-3	1	3	175.6	0.6
3	3	3	39.3	1.6
-3	3	3	146.8	1.0
3	5	3	168.1	2.0
-3	5	3	163.6	1.0
3	7	3	122.6	2.6
-3	7	3	190.3	1.0
3	9	3	193.7	1.6
-3	9	3	310.1	2.4
3	11	3	73.2	0.8
-3	11	3	19.8	5.9
3	13	3	34.3	0.9
-3	13	3	222.2	0.8
3	15	3	14.2	5.8
-3	15	3	126.2	1.3
3	17	3	65.7	0.8
-3	17	3	29.3	1.1
3	19	3	52.1	1.0
-3	19	3	29.3	1.5
3	21	3	30.4	2.7
-3	21	3	55.8	2.4
-3	23	3	111.6	1.2
4	0	3	17.9	1.6
-4	0	3	77.3	0.8
4	2	3	295.8	1.2
-4	2	3	33.6	1.5
4	4	3	83.5	1.4
-4	4	3	38.2	1.5
4	6	3	332.6	1.6
-4	6	3	119.7	0.7
4	8	3	45.3	1.1
-4	8	3	1.9	5.2
4	10	3	134.1	3.0
-4	10	3	190.9	3.0
4	12	3	112.9	0.8
-4	12	3	122.5	1.5
4	14	3	41.0	1.0
-4	14	3	125.9	1.6
4	16	3	198.8	1.6
-4	16	3	211.5	1.6
4	18	3	325.3	2.0
-4	18	3	206.0	2.2
4	20	3	118.0	2.1
-4	20	3	97.9	0.9
-4	22	3	43.6	1.1
5	1	3	9.6	2.4
-5	1	3	44.5	1.0
5	3	3	295.0	1.2
-5	3	3	279.9	1.2
5	5	3	362.9	3.2
-5	5	3	478.5	2.0
5	7	3	56.9	0.7
-5	7	3	115.5	2.2
5	9	3	131.0	0.7
-5	9	3	22.1	1.9
5	11	3	84.9	1.4
-5	11	3	72.4	0.7
5	13	3	61.3	1.5
-5	13	3	123.4	2.2
5	15	3	117.7	3.1
-5	15	3	194.3	1.0
5	17	3	154.5	1.8
-5	17	3	398.7	0.8
5	19	3	20.0	4.4
-5	19	3	175.7	2.8
-5	21	3	219.4	3.2
6	0	3	149.9	1.0
-6	0	3	136.5	0.8
6	2	3	28.1	3.7
-6	2	3	218.0	0.8
6	4	3	14.6	3.5
-6	4	3	18.7	7.3
6	6	3	627.7	5.6
-6	6	3	52.4	0.7
6	8	3	73.9	0.7
-6	8	3	34.4	1.3
6	10	3	43.1	1.0
-6	10	3	27.8	1.5
6	12	3	23.9	1.5
-6	12	3	84.6	3.6
6	14	3	251.2	1.2
-6	14	3	16.2	2.5
6	16	3	237.1	1.0
-6	16	3	166.8	3.0
6	18	3	346.9	3.6
-6	18	3	227.0	1.0
-6	20	3	136.3	2.8

## fluoro-tremolite 1082\_751\_361.cif

7	1	3	66.9	1.9
-7	1	3	81.8	2.3
7	3	3	42.3	2.6
-7	3	3	15.1	1.9
7	5	3	137.9	2.2
-7	5	3	102.9	1.9
7	7	3	55.6	1.4
-7	7	3	319.0	1.2
7	9	3	196.2	1.0
-7	9	3	200.6	2.0
7	11	3	73.8	1.2
-7	11	3	115.3	0.9
7	13	3	83.2	1.0
-7	13	3	188.6	1.4
7	15	3	63.2	1.8
-7	15	3	75.2	1.7
-7	17	3	210.0	1.0
-7	19	3	156.8	1.6
8	0	3	15.0	2.1
-8	0	3	98.8	1.0
8	2	3	88.9	0.9
-8	2	3	24.1	1.5
8	4	3	59.0	1.0
-8	4	3	107.1	2.0
8	6	3	196.1	1.8
-8	6	3	549.1	0.8
8	8	3	71.1	0.9
-8	8	3	131.1	1.2
8	10	3	28.6	2.6
-8	10	3	17.9	8.0
8	12	3	113.3	1.5
-8	12	3	59.3	1.0
8	14	3	13.2	11.0
-8	14	3	272.9	1.2
-8	16	3	195.8	3.4
-8	18	3	291.5	1.6
9	1	3	15.6	4.9
-9	1	3	24.4	4.4
9	3	3	162.3	1.2
-9	3	3	196.1	1.2
9	5	3	440.6	1.6
-9	5	3	517.2	2.4
9	7	3	177.9	1.4
-9	7	3	195.0	0.8
9	9	3	42.3	1.2
-9	9	3	30.4	1.0
9	11	3	0.0	12.4
-9	11	3	108.0	1.2
-9	13	3	20.4	7.9
-9	15	3	76.8	2.7
-9	17	3	337.3	3.2
10	0	3	105.4	1.4
-10	0	3	110.7	1.1
10	2	3	29.2	6.0
-10	2	3	178.5	0.8
10	4	3	56.2	1.3
-10	4	3	41.1	0.9
10	6	3	83.0	1.0
-10	6	3	46.7	3.5
10	8	3	103.3	1.5
-10	8	3	3.4	4.4
-10	10	3	16.0	7.4
-10	12	3	48.9	1.1
-10	14	3	41.9	2.4
-10	16	3	130.9	3.1
-11	1	3	95.2	1.6
-11	3	3	72.2	1.8
-11	5	3	249.7	1.2
-11	7	3	12.8	8.2
-11	9	3	88.6	0.9
-11	11	3	32.5	1.4
-11	13	3	52.0	1.1
-12	0	3	20.8	2.7
-12	2	3	126.9	2.0
-12	4	3	66.9	1.5
-12	6	3	453.3	5.6
-12	8	3	30.8	1.3
-12	10	3	182.0	4.0
-13	1	3	42.3	1.1
-13	3	3	15.4	8.3
-13	5	3	69.8	0.9
-13	7	3	83.6	1.2
0	0	4	568.0	0.8
0	2	4	81.2	0.6
0	4	4	165.2	1.2
0	6	4	63.3	1.4
0	8	4	189.4	0.8
0	10	4	202.3	0.8
0	12	4	441.9	1.2
0	14	4	29.1	2.0
0	16	4	148.3	1.0
0	18	4	86.4	1.0
0	20	4	115.0	1.3
1	1	4	53.7	6.6
-1	1	4	524.9	0.8
1	3	4	174.7	2.0

## fluoro-tremolite 1082\_751\_361.cif

-1	3	4	313.2	0.8
1	5	4	32.0	1.1
-1	5	4	203.5	0.8
1	7	4	176.2	2.0
-1	7	4	153.6	1.0
1	9	4	28.1	1.3
-1	9	4	220.9	2.2
1	11	4	114.4	0.9
-1	11	4	506.4	1.2
1	13	4	132.7	1.8
-1	13	4	92.8	0.7
1	15	4	118.2	1.0
-1	15	4	64.6	1.4
1	17	4	14.8	2.5
-1	17	4	78.1	1.9
1	19	4	49.2	1.0
-1	19	4	188.3	2.8
-1	21	4	23.5	1.7
2	0	4	713.4	0.8
-2	0	4	259.6	1.0
2	2	4	137.1	2.2
-2	2	4	98.2	0.8
2	4	4	35.9	1.9
-2	4	4	179.2	0.8
2	6	4	11.6	2.8
-2	6	4	8.6	3.9
2	8	4	100.8	0.7
-2	8	4	17.3	7.3
2	10	4	115.6	0.9
-2	10	4	71.9	2.4
2	12	4	229.4	1.2
-2	12	4	287.5	2.4
2	14	4	16.2	9.8
-2	14	4	126.2	1.9
2	16	4	29.2	3.0
-2	16	4	123.6	0.9
2	18	4	108.6	1.7
-2	18	4	132.1	2.4
2	20	4	141.6	1.0
-2	20	4	21.9	5.8
3	1	4	345.0	1.2
-3	1	4	253.2	1.8
3	3	4	43.5	5.2
-3	3	4	299.4	3.2
3	5	4	46.0	0.8
-3	5	4	17.4	1.5
3	7	4	90.3	0.9
-3	7	4	129.3	1.1
3	9	4	301.4	2.0
-3	9	4	19.5	1.0
3	11	4	606.8	0.8
-3	11	4	27.9	0.9
3	13	4	207.5	1.0
-3	13	4	167.5	1.6
3	15	4	142.9	1.8
-3	15	4	127.8	0.9
3	17	4	38.0	1.8
-3	17	4	10.6	4.8
3	19	4	102.7	3.1
-3	19	4	56.6	0.9
-3	21	4	167.5	1.6
4	0	4	73.0	1.1
-4	0	4	716.3	3.2
4	2	4	27.0	1.9
-4	2	4	118.8	0.7
4	4	4	86.7	1.0
-4	4	4	245.3	2.0
4	6	4	91.6	1.3
-4	6	4	25.9	2.2
4	8	4	55.6	1.4
-4	8	4	79.9	1.6
4	10	4	88.4	1.6
-4	10	4	146.4	2.2
4	12	4	213.7	2.2
-4	12	4	186.5	0.8
4	14	4	140.2	1.6
-4	14	4	46.6	1.1
4	16	4	86.3	1.8
-4	16	4	99.5	1.0
4	18	4	32.4	2.7
-4	18	4	79.9	1.0
-4	20	4	293.0	0.8
5	1	4	92.9	1.8
-5	1	4	37.4	0.8
5	3	4	101.4	2.0
-5	3	4	28.0	1.1
5	5	4	39.7	1.1
-5	5	4	83.8	1.1
5	7	4	256.3	1.0
-5	7	4	12.1	2.7
5	9	4	80.6	1.5
-5	9	4	252.4	1.0
5	11	4	111.3	1.7
-5	11	4	324.6	3.2
5	13	4	224.7	2.2
-5	13	4	13.2	2.0

## fluoro-tremolite 1082\_751\_361.cif

5	15	4	173.2	3.4
-5	15	4	50.5	0.9
-5	17	4	61.8	0.9
-5	19	4	62.8	0.9
6	0	4	268.9	1.2
-6	0	4	57.1	1.1
6	2	4	80.9	1.7
-6	2	4	137.3	0.8
6	4	4	28.6	3.8
-6	4	4	395.0	3.2
6	6	4	45.9	3.2
-6	6	4	66.6	1.2
6	8	4	271.7	1.6
-6	8	4	227.2	1.2
6	10	4	109.7	2.4
-6	10	4	43.2	0.8
6	12	4	239.0	3.2
-6	12	4	94.7	0.7
6	14	4	4.1	7.4
-6	14	4	67.9	0.9
-6	16	4	48.9	1.1
-6	18	4	104.5	0.9
7	1	4	124.6	1.2
-7	1	4	406.5	0.8
7	3	4	57.1	0.9
-7	3	4	170.4	1.6
7	5	4	151.8	1.4
-7	5	4	128.1	0.8
7	7	4	4.3	5.7
-7	7	4	208.6	1.0
7	9	4	118.6	1.0
-7	9	4	130.0	0.8
7	11	4	187.1	2.6
-7	11	4	377.6	2.4
7	13	4	25.6	11.1
-7	13	4	16.0	4.2
-7	15	4	22.1	4.5
-7	17	4	74.3	1.0
-7	19	4	90.6	1.3
8	0	4	83.1	1.3
-8	0	4	659.9	0.8
8	2	4	82.6	1.0
-8	2	4	93.8	3.3
8	4	4	144.6	1.4
-8	4	4	53.6	1.2
8	6	4	28.7	3.3
-8	6	4	53.5	1.7
8	8	4	218.6	1.8
-8	8	4	351.5	1.6
8	10	4	18.6	2.2
-8	10	4	185.1	0.8
-8	12	4	508.4	1.2
-8	14	4	17.3	17.4
-8	16	4	255.7	2.6
9	1	4	73.5	1.7
-9	1	4	46.0	1.2
9	3	4	12.8	12.9
-9	3	4	167.6	0.8
9	5	4	89.0	1.1
-9	5	4	37.8	1.0
-9	7	4	130.2	1.0
-9	9	4	12.6	2.4
-9	11	4	178.3	2.0
-9	13	4	43.0	1.1
-9	15	4	106.6	2.9
-10	0	4	103.0	1.2
-10	2	4	25.5	1.3
-10	4	4	22.7	1.8
-10	6	4	63.5	1.6
-10	8	4	142.4	1.0
-10	10	4	97.6	0.9
-10	12	4	226.4	1.2
-10	14	4	136.4	2.6
-11	1	4	103.9	1.9
-11	3	4	54.8	1.4
-11	5	4	50.8	0.9
-11	7	4	54.8	1.0
-11	9	4	275.7	1.6
-11	11	4	344.5	3.2
-12	0	4	211.4	2.0
-12	2	4	62.6	1.0
-12	4	4	65.8	1.9
-12	6	4	98.1	1.8
-12	8	4	14.6	3.0
-13	1	4	117.8	1.0
-13	3	4	111.4	1.4
0	0	5	70.8	1.2
0	2	5	194.2	0.8
0	4	5	14.5	3.1
0	6	5	343.3	0.8
0	8	5	45.2	4.0
0	10	5	170.5	1.6
0	12	5	67.0	1.4
0	14	5	404.5	1.2
0	16	5	227.9	1.8
0	18	5	159.1	2.4

## fluoro-tremolite 1082\_751\_361.cif

1	1	5	34.1	1.2
-1	1	5	68.1	0.7
1	3	5	34.7	1.6
-1	3	5	14.8	5.2
1	5	5	157.7	1.0
-1	5	5	102.1	0.7
1	7	5	29.8	2.1
-1	7	5	134.8	0.8
1	9	5	119.2	1.3
-1	9	5	109.8	0.9
1	11	5	110.0	0.8
-1	11	5	44.2	1.3
1	13	5	71.8	0.9
-1	13	5	139.7	2.8
1	15	5	52.9	1.0
-1	15	5	28.9	1.3
1	17	5	36.0	2.0
-1	17	5	45.0	3.2
2	0	5	45.5	1.3
-2	0	5	91.2	1.0
2	2	5	243.3	0.8
-2	2	5	292.4	1.6
2	4	5	29.8	3.8
-2	4	5	81.7	1.6
2	6	5	25.1	1.7
-2	6	5	211.8	1.2
2	8	5	30.5	1.5
-2	8	5	42.8	1.6
2	10	5	91.4	1.3
-2	10	5	96.4	0.9
2	12	5	125.6	0.8
-2	12	5	51.4	0.9
2	14	5	86.2	1.0
-2	14	5	114.3	0.8
2	16	5	98.0	0.9
-2	16	5	101.6	1.5
-2	18	5	325.5	2.0
3	1	5	14.8	5.5
-3	1	5	60.9	0.7
3	3	5	258.4	1.8
-3	3	5	210.8	1.4
3	5	5	418.7	1.2
-3	5	5	380.1	2.8
3	7	5	126.6	1.9
-3	7	5	52.5	1.6
3	9	5	79.9	1.6
-3	9	5	9.7	4.1
3	11	5	14.8	3.1
-3	11	5	91.0	1.3
3	13	5	56.9	2.8
-3	13	5	78.6	2.2
3	15	5	189.7	1.8
-3	15	5	165.7	1.6
-3	17	5	312.3	1.2
4	0	5	121.1	1.2
-4	0	5	116.4	1.0
4	2	5	25.5	6.4
-4	2	5	14.2	9.4
4	4	5	0.0	5.8
-4	4	5	20.7	5.7
4	6	5	564.0	3.2
-4	6	5	671.0	0.8
4	8	5	13.7	3.0
-4	8	5	92.7	0.7
4	10	5	97.7	1.1
-4	10	5	94.9	2.3
4	12	5	22.4	1.7
-4	12	5	62.2	0.9
4	14	5	118.0	1.5
-4	14	5	140.2	1.0
-4	16	5	223.3	2.4
-4	18	5	233.5	1.8
5	1	5	47.5	1.4
-5	1	5	118.4	1.1
5	3	5	115.2	0.8
-5	3	5	33.6	4.3
5	5	5	80.0	3.6
-5	5	5	143.8	1.0
5	7	5	103.2	0.9
-5	7	5	85.1	1.1
5	9	5	186.0	3.4
-5	9	5	205.0	1.0
5	11	5	48.8	1.0
-5	11	5	52.7	0.8
-5	13	5	148.6	1.8
-5	15	5	72.5	0.9
-5	17	5	51.4	1.3
6	0	5	0.0	6.2
-6	0	5	75.7	1.1
6	2	5	63.8	1.0
-6	2	5	75.7	1.0
6	4	5	50.2	2.3
-6	4	5	21.5	1.6
6	6	5	15.9	10.9
-6	6	5	184.5	0.8
6	8	5	20.8	4.4

## fluoro-tremolite 1082\_751\_361.cif

-6	8	5	26.7	3.6
-6	10	5	14.0	2.2
-6	12	5	85.1	0.8
-6	14	5	164.3	3.2
-6	16	5	186.5	1.4
7	1	5	22.1	1.8
-7	1	5	29.6	3.4
7	3	5	157.6	4.4
-7	3	5	251.9	3.0
7	5	5	281.5	1.2
-7	5	5	550.2	2.4
-7	7	5	253.1	1.4
-7	9	5	115.6	1.2
-7	11	5	94.1	1.3
-7	13	5	15.4	2.3
-7	15	5	91.6	2.6
-8	0	5	57.3	1.2
-8	2	5	57.6	1.1
-8	4	5	17.9	1.6
-8	6	5	56.0	7.7
-8	8	5	60.4	0.9
-8	10	5	45.6	3.6
-8	12	5	69.5	0.9
-8	14	5	110.0	0.9
-9	1	5	59.1	1.9
-9	3	5	83.8	1.4
-9	5	5	143.8	1.8
-9	7	5	306.1	1.6
-9	9	5	233.3	1.0
-9	11	5	43.1	1.3
-9	13	5	91.9	0.9
-10	0	5	66.1	1.3
-10	2	5	41.7	9.2
-10	4	5	75.1	2.3
-10	6	5	273.2	2.0
-10	8	5	64.4	1.2
-10	10	5	66.2	4.1
-11	1	5	27.4	1.3
-11	3	5	153.1	1.0
-11	5	5	268.1	1.0
-11	7	5	37.0	1.5
-11	9	5	13.2	3.8
-12	0	5	146.0	1.4
-12	2	5	191.7	1.6
-12	4	5	90.7	1.7
0	0	6	204.7	1.2
0	2	6	97.5	0.8
0	4	6	123.4	1.7
0	6	6	3.6	6.0
0	8	6	145.0	1.0
0	10	6	72.4	1.3
0	12	6	178.3	1.4
1	1	6	268.4	1.0
-1	1	6	102.4	0.9
1	3	6	124.4	2.0
-1	3	6	150.6	2.2
1	5	6	154.3	1.4
-1	5	6	54.6	1.1
1	7	6	71.3	1.9
-1	7	6	159.3	1.6
1	9	6	100.8	1.0
-1	9	6	38.8	2.0
1	11	6	253.6	1.2
-1	11	6	6.7	8.3
1	13	6	24.8	1.6
-1	13	6	180.4	1.6
2	0	6	177.5	1.2
-2	0	6	535.3	1.2
2	2	6	29.4	2.2
-2	2	6	73.5	0.9
2	4	6	99.3	1.2
-2	4	6	15.8	2.1
2	6	6	55.7	1.4
-2	6	6	58.5	1.5
2	8	6	55.5	1.5
-2	8	6	82.7	1.0
2	10	6	58.2	2.2
-2	10	6	106.3	0.9
-2	12	6	198.5	1.8
-2	14	6	51.6	2.9
3	1	6	139.9	3.2
-3	1	6	330.8	1.2
3	3	6	123.5	0.9
-3	3	6	99.8	1.4
3	5	6	69.0	1.0
-3	5	6	18.2	11.3
3	7	6	88.3	5.3
-3	7	6	62.7	1.1
3	9	6	90.5	0.9
-3	9	6	323.3	1.6
-3	11	6	590.2	1.6
-3	13	6	211.4	3.0
4	0	6	564.8	1.6
-4	0	6	199.9	1.2
4	2	6	83.3	1.1
-4	2	6	68.5	1.1

## fluoro-tremolite 1082\_751\_361.cif

4	4	6	142.1	1.0
-4	4	6	37.1	3.2
4	6	6	31.8	1.4
-4	6	6	9.7	8.9
-4	8	6	53.1	0.9
-4	10	6	90.3	1.8
-4	12	6	62.3	1.2
-4	14	6	57.5	1.3
-5	1	6	11.7	2.4
-5	3	6	117.0	0.7
-5	5	6	46.2	1.0
-5	7	6	206.2	2.0
-5	9	6	48.3	2.6
-5	11	6	19.0	2.0
-5	13	6	117.6	0.9
-6	0	6	263.6	1.2
-6	2	6	57.5	1.3
-6	4	6	21.6	1.8
-6	6	6	10.4	5.5
-6	8	6	277.3	1.2
-6	10	6	135.1	1.2
-6	12	6	224.7	3.4
-7	1	6	97.6	1.1
-7	3	6	69.1	0.9
-7	5	6	151.1	2.8
-7	7	6	67.1	1.8
-7	9	6	107.1	1.0
-7	11	6	138.6	3.2
-8	0	6	76.8	1.3
-8	2	6	94.7	1.1
-8	4	6	220.4	1.2
-8	6	6	47.7	4.5
-8	8	6	232.2	1.4
-8	10	6	4.0	9.1
-9	1	6	20.8	5.4
-9	3	6	71.8	3.3
-9	5	6	18.3	4.0
-9	7	6	34.3	2.4
-9	9	6	168.1	1.0
-10	0	6	584.8	1.6
-10	2	6	124.1	3.0
-10	4	6	117.1	0.9
-10	6	6	63.4	2.5
0	0	7	13.4	3.6
0	2	7	193.3	1.6
0	4	7	57.2	2.3
1	1	7	21.5	11.6
-1	1	7	9.0	8.5
-1	3	7	8.1	4.9
-1	5	7	166.0	1.4
-1	7	7	38.0	1.8
-2	0	7	49.2	1.6
-2	2	7	136.4	1.2
-2	4	7	16.5	4.8
-2	6	7	437.2	0.8
-2	8	7	33.1	1.3
-3	1	7	66.5	1.9
-3	3	7	62.8	1.3
-3	5	7	137.6	1.4
-3	7	7	28.9	1.5
-4	0	7	79.5	1.3
-4	2	7	175.8	2.8
-4	4	7	22.0	4.6
-4	6	7	250.8	1.8
-4	8	7	20.3	1.9
-5	1	7	24.2	1.7
-5	3	7	116.6	0.9
-5	5	7	162.0	1.6
-5	7	7	20.4	4.6
-6	0	7	80.8	1.3
-6	2	7	19.2	5.1
-6	4	7	57.1	2.5
-6	6	7	319.9	2.4
-7	1	7	36.6	2.4
-7	3	7	35.0	1.7