Helium Cryostat Synchrotron Charge Densities Using a Large CCD Detector – The Upgraded Beam Line D3 at DESY*

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Contents:

CIF FILE

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##CIF_1.1

#  Archive CIF produced by XD routine XDCIF
#  Created on 2008-05-19 at 08:42:37
#  Using CIFtbx version 2.6.2 16 Jun 1998

#  Dictionary name : cif_core.dic
#  Dictionary vers : 2.2
#  Request file    : /home/jacobo/xd/xd2006/lib/xd/xdcif.dat
#  CIF files read  : fft geo lsm



_audit_creation_date            2008-05-19T08:42:37-00:00
_audit_creation_method         'XD routine XDCIF'
_audit_conform_dict_name        cif_core.dic
_audit_conform_dict_version     2.2
_audit_conform_dict_location    ftp://ftp.iucr.org/pub/cif_core.dic

#------------------------------------------------------------------------------#
#                    CHEMICAL INFORMATION                                      #
#------------------------------------------------------------------------------#


#------------------------------------------------------------------------------#
#                    UNIT CELL INFORMATION                                     #
#------------------------------------------------------------------------------#

loop_
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    _space_group_symop_operation_xyz
1 +X,+Y,+Z
2 -X,-Y,-Z

_cell_length_a                          6.2170(10)
_cell_length_b                          6.9850(10)
_cell_length_c                          10.5060(10)
_cell_angle_alpha                       94.686
_cell_angle_beta                        100.568(2)
_cell_angle_gamma                       98.884
_cell_volume                            440.26(10)

#------------------------------------------------------------------------------#
#                    CRYSTAL INFORMATION                                       #
#------------------------------------------------------------------------------#


#------------------------------------------------------------------------------#
#                    ABSORPTION CORRECTION                                     #
#------------------------------------------------------------------------------#

_exptl_absorpt_correction_type          none

#------------------------------------------------------------------------------#
#                    DATA COLLECTION                                           #
#------------------------------------------------------------------------------#


#------------------------------------------------------------------------------#
#                    COMPUTER PROGRAMS USED                                    #
#------------------------------------------------------------------------------#

_computing_structure_refinement         'Volkov et al, (2006)'
_computing_molecular_graphics           'Volkov et al, (2006)'
```

```
_computing_publication_material         'Volkov et al, (2006)'

#------------------------------------------------------------------------------#
#                    REFINEMENT INFORMATION                                    #
#------------------------------------------------------------------------------#

_refine_special_details
;
        ?
;
_refine_ls_structure_factor_coef        Fsqd
_refine_ls_matrix_type                  full
_refine_ls_weighting_scheme             calc
_refine_ls_weighting_details
;
        calc w2 = 1/[s^2^(Fo^2^)]
;
_refine_ls_extinction_method            none
_refine_ls_number_reflns                8807
_refine_ls_number_parameters            348
_refine_ls_number_restraints            0
_refine_ls_R_factor_all                 0.031
_refine_ls_R_factor_gt                  0.026
_refine_ls_wR_factor_ref                0.033
_refine_ls_goodness_of_fit_ref          1.293
_refine_ls_shift/su_max                 0
_refine_diff_density_max                0.414
_refine_diff_density_min                -0.507
_refine_diff_density_rms                0.099

#------------------------------------------------------------------------------#
#                    ATOMIC TYPES, COORDINATES AND THERMAL PARAMETERS          #
#------------------------------------------------------------------------------#

loop_
    _atom_site_label
    _atom_site_fract_x
    _atom_site_fract_y
    _atom_site_fract_z
    _atom_site_U_iso_or_equiv
    _atom_site_occupancy
    _atom_site_symmetry_multiplicity
K(1) 0.166902(10) 0.146531(9) 0.272299(6) 0.005 1 2
O(1) 0.32768(6) 0.32887(5) 0.06605(3) 0.005 1 2
O(2) -0.49600(6) -0.07104(5) 0.15539(3) 0.005 1 2
O(3) 0.65294(6) 0.51936(5) 0.15900(3) 0.005 1 2
O(4) -0.23141(6) 0.11365(5) 0.07737(3) 0.005 1 2
O(5) 0.18091(6) -0.44219(5) 0.30600(3) 0.006 1 2
O(6) 0.28126(6) -0.15314(5) 0.42892(3) 0.006 1 2
O(7) 0.35630(6) -0.34409(5) 0.64478(3) 0.006 1 2
O(8) 0.21781(6) -0.62730(5) 0.51715(3) 0.006 1 2
O(9) -0.21285(6) -0.05175(5) 0.35666(3) 0.006 1 2
O(10) 0.05496(6) -0.23947(5) 0.12958(3) 0.006 1 2
C(1) 0.48896(5) 0.45360(5) 0.06365(3) 0.004 1 2
C(2) -0.41627(5) 0.01568(5) 0.06547(3) 0.004 1 2
C(3) 0.24662(5) -0.33147(5) 0.41668(3) 0.004 1 2
C(4) 0.27615(5) -0.44739(5) 0.53688(3) 0.004 1 2
H(2) -0.37051 -0.060957 0.243925 0.014 1 2
H(3) 0.643304 0.443508 0.247473 0.016 1 2
H(5) 0.137889 -0.357491 0.22923 0.015 1 2
H(9A) -0.214791 -0.179727 0.389357 0.017 1 2
H(9B) -0.252828 0.033091 0.424914 0.017 1 2
H(10A) 0.142382 -0.202357 0.064608 0.018 1 2
H(10B) -0.094466 -0.290244 0.081178 0.019 1 2

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    _atom_site_aniso_label
    _atom_site_aniso_U_11
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    _atom_site_aniso_U_22
    _atom_site_aniso_U_33
    _atom_site_aniso_U_23
    _atom_site_aniso_U_13
    _atom_site_aniso_U_12
K(1) 0.00580(6) 0.00486(6) 0.00548(6) 0.00075(4) 0.00117(4) -0.00018(4)
O(1) 0.00492(10) 0.00590(10) 0.00412(10) 0.00131(8) 0.00006(8) -0.00124(9)
O(2) 0.00534(10) 0.00783(11) 0.00281(10) 0.00221(8) -0.00020(8) 0.00008(9)
O(3) 0.00589(11) 0.00639(10) 0.00255(9) 0.00151(8) -0.00129(8) -0.00078(9)
O(4) 0.00407(10) 0.00692(10) 0.00415(10) 0.00110(8) -0.00043(8) -0.00080(9)
O(5) 0.01056(12) 0.00447(10) 0.00202(9) 0.00014(8) -0.00066(8) 0.00162(9)
O(6) 0.00916(11) 0.00319(9) 0.00390(10) 0.00057(8) 0.00042(8) 0.00083(9)
O(7) 0.00869(11) 0.00503(10) 0.00201(9) 0.00039(8) -0.00072(8) 0.00022(9)
O(8) 0.01088(12) 0.00320(10) 0.00404(10) 0.00082(8) 0.00033(9) 0.00093(9)
O(9) 0.00744(11) 0.00578(10) 0.00342(10) 0.00092(8) 0.00017(8) 0.00201(9)
O(10) 0.00519(10) 0.00768(11) 0.00403(10) 0.00195(8) -0.00021(8) 0.00022(9)
C(1) 0.00434(10) 0.00406(9) 0.00242(9) 0.00071(7) -0.00017(8) 0.00007(9)
C(2) 0.00385(10) 0.00468(9) 0.00258(9) 0.00070(8) -0.00020(7) 0.00031(9)
C(3) 0.00560(10) 0.00338(10) 0.00237(9) 0.00060(8) 0.00018(8) 0.00080(8)
C(4) 0.00558(10) 0.00341(10) 0.00235(9) 0.00067(8) 0.00012(8) 0.00098(8)
H(2) 0.016856 0.015465 0.010833 0.002567 0.002878 0.001305
H(3) 0.017916 0.014655 0.012989 0.001235 0.002267 0.000409
H(5) 0.021878 0.01346 0.009357 0.002375 0.002341 0.002214
H(9A) 0.02769 0.011247 0.014467 0.005786 0.003393 0.005424
H(9B) 0.02526 0.016044 0.011832 -0.001987 0.005609 0.005915
H(10A) 0.021866 0.020196 0.01426 0.005935 0.010276 0.000856
H(10B) 0.012474 0.021665 0.018989 0.000645 -0.002242 -0.002279

loop_
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    _atom_site_anharm_GC_D_3333
    _atom_site_anharm_GC_D_1112
    _atom_site_anharm_GC_D_1222
    _atom_site_anharm_GC_D_1113
    _atom_site_anharm_GC_D_1333
    _atom_site_anharm_GC_D_2223
    _atom_site_anharm_GC_D_2333
    _atom_site_anharm_GC_D_1122
    _atom_site_anharm_GC_D_1133
    _atom_site_anharm_GC_D_2233
    _atom_site_anharm_GC_D_1123
    _atom_site_anharm_GC_D_1223
    _atom_site_anharm_GC_D_1233
K(1) 0.000139(52) 0.000327(28) 0.000127(6) -0.000428(25) -0.000264(16) 0.000384(14)
0.000027(5) 0.000095(9)
0.000007(4) -0.000129(17) 0.000164(7) 0.000111(5) 0.000138(7) 0.000082(6)
0.000038(4)


#------------------------------------------------------------------------------#
#                    MULTIPOLE PARAMETERS                                      #
#------------------------------------------------------------------------------#


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_atom_rho_multipole_coeff_P1-1
_atom_rho_multipole_coeff_P10
_atom_rho_multipole_coeff_P20
_atom_rho_multipole_coeff_P21
_atom_rho_multipole_coeff_P2-1
_atom_rho_multipole_coeff_P22
_atom_rho_multipole_coeff_P2-2
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```
_atom_rho_multipole_coeff_P30
_atom_rho_multipole_coeff_P31
_atom_rho_multipole_coeff_P3-1
_atom_rho_multipole_coeff_P32
_atom_rho_multipole_coeff_P3-2
_atom_rho_multipole_coeff_P33
_atom_rho_multipole_coeff_P3-3
_atom_rho_multipole_coeff_P40
_atom_rho_multipole_coeff_P41
_atom_rho_multipole_coeff_P4-1
_atom_rho_multipole_coeff_P42
_atom_rho_multipole_coeff_P4-2
_atom_rho_multipole_coeff_P43
_atom_rho_multipole_coeff_P4-3
_atom_rho_multipole_coeff_P44
_atom_rho_multipole_coeff_P4-4
_atom_rho_multipole_kappa
_atom_rho_multipole_kappa_prime0
_atom_rho_multipole_kappa_prime1
_atom_rho_multipole_kappa_prime2
_atom_rho_multipole_kappa_prime3
_atom_rho_multipole_kappa_prime4
_atom_rho_multipole_radial_slater_n0
_atom_rho_multipole_radial_slater_zeta0
_atom_rho_multipole_radial_slater_n1
_atom_rho_multipole_radial_slater_zeta1
_atom_rho_multipole_radial_slater_n2
_atom_rho_multipole_radial_slater_zeta2
_atom_rho_multipole_radial_slater_n3
_atom_rho_multipole_radial_slater_zeta3
_atom_rho_multipole_radial_slater_n4
_atom_rho_multipole_radial_slater_zeta4
K(1) 18 0 0 0 0
0 0 0 0 0
0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1
0 0 0 0 0 0 0 0 0 0 0

O(1) 6.383(17) 0 -0.034(10) 0.010(8) 0.004(8)
-0.093(9) -0.005(8) 0.001(8) -0.065(9) 0.025(8)
-0.017(8) -0.016(8) 0.001(7) -0.009(7) 0.008(7) 0.041(7) -0.006(7)
0 0 0 0 0 0 0 0 0
0.9723(10) 0.955911 0.955911 0.955911 0.955911 0.955911
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

O(2) 6.426(19) 0 0.020(9) -0.039(9) 0.002(9)
-0.013(9) -0.001(9) -0.012(8) 0.089(9) -0.008(9)
-0.007(8) -0.031(8) -0.026(8) -0.010(8) -0.006(7) 0.088(7) -0.021(8)
0 0 0 0 0 0 0 0 0
0.9742(12) 0.957394 0.957394 0.957394 0.957394 0.957394
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

O(3) 6.371(19) 0 0.014(9) -0.062(9) 0.007(9)
-0.037(9) -0.009(9) -0.005(8) 0.063(8) -0.009(9)
0.009(8) -0.029(8) -0.014(8) -0.003(7) 0.003(7) 0.095(7) -0.009(7)
0 0 0 0 0 0 0 0 0
0.9742(12) 0.957394 0.957394 0.957394 0.957394 0.957394
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

O(4) 6.348(17) 0 -0.045(10) -0.002(8) 0.004(8)
-0.083(9) 0.011(8) -0.007(8) -0.067(9) -0.029(8)
-0.005(8) -0.004(8) -0.001(8) -0.001(7) 0.006(7) 0.054(7) -0.002(7)
0 0 0 0 0 0 0 0 0
0.9723(10) 0.955911 0.955911 0.955911 0.955911 0.955911
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

O(5) 6.40(2) 0 -0.011(9) -0.033(9) 0.003(9)
```

```
-0.052(9) -0.014(9) -0.011(9) 0.048(9) -0.004(9)
-0.001(8) -0.023(8) -0.017(8) -0.009(8) 0.007(8) 0.100(8) -0.020(8)
0 0 0 0 0 0 0 0 0
0.9742(12) 0.957394 0.957394 0.957394 0.957394 0.957394
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

O(6) 6.387(17) 0 -0.049(9) -0.005(8) -0.006(8)
-0.102(9) 0.032(9) -0.011(8) -0.064(8) 0.006(8)
-0.005(8) -0.002(8) -0.019(7) 0.007(8) -0.008(7) 0.047(7) -0.003(7)
0 0 0 0 0 0 0 0 0
0.9723(10) 0.955911 0.955911 0.955911 0.955911 0.955911
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

O(7) 6.423(17) 0 -0.042(9) -0.012(8) -0.009(8)
-0.079(9) -0.002(9) -0.022(8) -0.031(9) -0.040(8)
0.002(8) -0.013(8) 0.001(7) -0.013(8) -0.002(7) 0.071(7) -0.012(7)
0 0 0 0 0 0 0 0 0
0.9723(10) 0.955911 0.955911 0.955911 0.955911 0.955911
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

O(8) 6.403(16) 0 -0.045(9) -0.012(8) -0.004(8)
-0.107(9) -0.048(9) 0.016(8) -0.078(8) 0.005(8)
0.006(8) -0.028(8) -0.006(7) -0.002(8) 0.008(7) 0.043(7) -0.004(7)
0 0 0 0 0 0 0 0 0
0.9723(10) 0.955911 0.955911 0.955911 0.955911 0.955911
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

O(9) 6.55(3) 0 -0.029(8) -0.028(8) 0.002(8)
0.001(9) -0.038(8) -0.017(8) -0.017(7) 0.016(8)
-0.002(8) -0.034(7) -0.054(7) -0.007(7) 0.016(7) 0.093(7) -0.037(7)
0 0 0 0 0 0 0 0 0
0.9645(16) 0.967312 0.967312 0.967312 0.967312 0.967312
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

O(10) 6.55(3) 0 -0.027(8) -0.031(8) 0.007(8)
0.013(9) -0.001(8) 0.012(8) -0.021(7) 0.043(8)
0.006(8) -0.033(7) -0.043(8) 0.008(7) -0.016(7) 0.109(7) -0.040(7)
0 0 0 0 0 0 0 0 0
0.9645(16) 0.967312 0.967312 0.967312 0.967312 0.967312
2 4.466 2 4.466 2 4.466 3 4.466 4 4.466

C(1) 3.83(2) 0 0.043(11) -0.018(9) -0.006(9)
-0.237(10) -0.003(9) -0.006(9) 0.007(11) -0.017(9)
0.008(12) 0.036(11) -0.003(10) -0.002(10) 0.014(11) 0.302(11) 0.010(13)
0 0 0 0 0 0 0 0 0
1.013(2) 1.001788 1.001788 1.001788 1.001788 1.001788
2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762

C(2) 3.80(2) 0 0.054(11) -0.008(9) 0.002(9)
-0.257(10) 0.007(9) -0.003(9) 0.027(11) 0.004(9)
0.007(12) 0.003(11) 0.010(10) -0.009(10) 0.028(11) 0.309(11) 0.018(14)
0 0 0 0 0 0 0 0 0
1.013(2) 1.001788 1.001788 1.001788 1.001788 1.001788
2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762

C(3) 3.79(2) 0 0.078(11) -0.044(10) 0.021(9)
-0.265(10) 0.016(9) 0.001(9) 0.031(10) 0.015(10)
-0.014(11) -0.007(11) 0.012(10) 0.003(11) 0.008(11) 0.294(12) -0.001(12)
0 0 0 0 0 0 0 0 0
1.013(2) 1.001788 1.001788 1.001788 1.001788 1.001788
2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762

C(4) 3.82(2) 0 0.032(11) 0.017(10) -0.007(8)
-0.245(10) -0.030(9) 0.004(9) 0.014(10) -0.036(10)
0.021(11) -0.002(11) -0.003(10) -0.011(11) -0.012(11) 0.293(12) 0.034(12)
0 0 0 0 0 0 0 0 0
1.013(2) 1.001788 1.001788 1.001788 1.001788 1.001788
2 3.1762 2 3.1762 2 3.1762 3 3.1762 4 3.1762
```

```
H(2) 0.579(13) 0 0.001(8) -0.004(8) 0.057(11)
0.037(16) 0.018(14) -0.042(14) -0.010(12) 0.003(12)
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 2 1 2 2 2 3 2 4 2

H(3) 0.593(12) 0 -0.016(9) 0.001(8) 0.023(10)
0.089(16) 0.015(14) 0.043(14) 0.017(12) -0.001(12)
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 2 1 2 2 2 3 2 4 2

H(5) 0.600(13) 0 0.017(8) -0.003(9) 0.101(11)
0.071(16) 0.037(13) -0.011(14) -0.014(12) 0.013(11)
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 2 1 2 2 2 3 2 4 2

H(9A) 0.689(9) 0 0 0 0.110(7)
0.069(8) 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 2 1 2 2 2 3 2 4 2

H(9B) 0.6885 0 0 0 0.1095
0.0688 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 2 1 2 2 2 3 2 4 2

H(10A) 0.6885 0 0 0 0.1095
0.0688 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 2 1 2 2 2 3 2 4 2

H(10B) 0.6885 0 0 0 0.1095
0.0688 0 0 0 0
0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0
1.2 1.2 1.2 1.2 1.2 1.2
0 2 1 2 2 2 3 2 4 2

loop_
    _atom_local_axes_atom_label
    _atom_local_axes_atom0
    _atom_local_axes_ax1
    _atom_local_axes_atom1
    _atom_local_axes_atom2
    _atom_local_axes_ax2
K(1) O(1) Z K(1) O(6) Y
O(1) C(1) X O(1) O(3) Y
O(2) H(2) X O(2) C(2) Y
O(3) H(3) X O(3) C(1) Y
O(4) C(2) X O(4) O(2) Y
O(5) H(5) X O(5) C(3) Y
O(6) C(3) X O(6) O(5) Y
O(7) C(4) X O(7) O(8) Y
O(8) C(4) X O(8) O(7) Y
O(9) H(9A) X O(9) H(9B) Y
O(10) H(10A) X O(10) H(10B) Y
```

```
C(1) O(1) X C(1) O(3) Y
C(2) O(4) X C(2) O(2) Y
C(3) O(6) X C(3) O(5) Y
C(4) O(8) X C(4) O(7) Y
H(2) O(2) Z H(2) O(9) Y
H(3) O(3) Z H(3) C(1) Y
H(5) O(5) Z H(5) O(10) Y
H(9A) O(9) Z H(9A) H(9B) Y
H(9B) O(9) Z H(9B) H(9A) Y
H(10A) O(10) Z H(10A) H(10B) Y
H(10B) O(10) Z H(10B) H(10A) Y


#------------------------------------------------------------------------------#
#                    MOLECULAR GEOMETRY                                        #
#------------------------------------------------------------------------------#

loop_
    _geom_bond_atom_site_label_1
    _geom_bond_atom_site_label_2
    _geom_bond_distance
    _geom_bond_site_symmetry_1
    _geom_bond_site_symmetry_2
    _geom_bond_publ_flag
O(1) C(1) 1.2281(4) 1_555 1_555 yes
O(2) C(2) 1.2952(4) 1_555 1_555 yes
O(2) H(2) 1.0885(3) 1_555 1_555 yes
O(3) C(1) 1.2882(4) 1_555 1_555 yes
O(3) H(3) 1.1133(3) 1_555 1_555 yes
O(4) C(2) 1.2228(4) 1_555 1_555 yes
O(5) C(3) 1.3033(4) 1_555 1_555 yes
O(5) H(5) 1.0582(3) 1_555 1_555 yes
O(6) C(3) 1.2229(4) 1_555 1_555 yes
O(7) C(4) 1.2657(4) 1_555 1_555 yes
O(7) H(3) 1.3754(3) 1_555 2_656 yes
O(8) C(4) 1.2421(4) 1_555 1_555 yes
O(9) H(2) 1.3820(3) 1_555 1_555 yes
O(9) H(9A) 0.9827(3) 1_555 1_555 yes
O(9) H(9B) 0.9842(3) 1_555 1_555 yes
O(10) H(5) 1.4546(3) 1_555 1_555 yes
O(10) H(10A) 0.9747(3) 1_555 1_555 yes
O(10) H(10B) 0.9710(3) 1_555 1_555 yes
C(1) C(1) 1.5521(6) 1_555 2_665 yes
C(2) C(2) 1.5425(6) 1_555 2_455 yes
C(3) C(4) 1.5530(4) 1_555 1_555 yes
H(9A) H(9B) 1.5670031389722 1_555 1_555 yes
H(10A) H(10B) 1.551664258724 1_555 1_555 yes

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_2
    _geom_angle_site_symmetry_3
    _geom_angle_publ_flag
C(2) O(2) H(2) 111.54(3) 1_555 1_555 1_555 yes
C(1) O(3) H(3) 112.99(3) 1_555 1_555 1_555 yes
C(3) O(5) H(5) 110.49(3) 1_555 1_555 1_555 yes
C(4) O(7) H(3) 114.80(3) 1_555 1_555 2_656 yes
H(2) O(9) H(9A) 111.54(3) 1_555 1_555 1_555 yes
H(2) O(9) H(9B) 108.01(3) 1_555 1_555 1_555 yes
H(9A) O(9) H(9B) 105.63(3) 1_555 1_555 1_555 yes
H(5) O(10) H(10A) 119.94(3) 1_555 1_555 1_555 yes
H(5) O(10) H(10B) 114.53(3) 1_555 1_555 1_555 yes
H(10A) O(10) H(10B) 105.78(3) 1_555 1_555 1_555 yes
O(1) C(1) O(3) 126.41(3) 1_555 1_555 1_555 yes
```

```
O(1) C(1) C(1) 120.25(4) 1_555 1_555 2_665 yes
O(3) C(1) C(1) 113.33(3) 1_555 1_555 2_665 yes
O(2) C(2) O(4) 126.43(3) 1_555 1_555 1_555 yes
O(2) C(2) C(2) 112.39(3) 1_555 1_555 2_455 yes
O(4) C(2) C(2) 121.18(4) 1_555 1_555 2_455 yes
O(5) C(3) O(6) 125.02(3) 1_555 1_555 1_555 yes
O(5) C(3) C(4) 113.58(3) 1_555 1_555 1_555 yes
O(6) C(3) C(4) 121.40(3) 1_555 1_555 1_555 yes
O(7) C(4) O(8) 127.74(3) 1_555 1_555 1_555 yes
O(7) C(4) C(3) 114.90(3) 1_555 1_555 1_555 yes
O(8) C(4) C(3) 117.36(3) 1_555 1_555 1_555 yes
O(2) H(2) O(9) 178.91(2) 1_555 1_555 1_555 yes
O(3) H(3) O(7) 176.05(2) 1_555 1_555 2_656 yes
O(5) H(5) O(10) 173.22(2) 1_555 1_555 1_555 yes
O(9) H(9A) H(9B) 37.22(2) 1_555 1_555 1_555 yes
O(9) H(9B) H(9A) 37.152(19) 1_555 1_555 1_555 yes
O(10) H(10A) H(10B) 37.03(2) 1_555 1_555 1_555 yes
O(10) H(10B) H(10A) 37.19(2) 1_555 1_555 1_555 yes
```

Output from UIJXN for D3 data

```
1PROGRAM UIJXN.  13:28:40  8-May-08.        OxHy2 XR/N/XResd/Nesd
0LEAST-SQUARES COMPARISON OF X-RAY AND NEUTRON THERMAL PARAMETERS
0ATOMIC DEBYE-WALLER FACTORS
0EXP(-M) = EXP(-2*PI**2*(SUM(I=1,3) SUM(J=1,3)
                          H(I)*H(J)*ASTAR(I)*ASTAR(J)*U(I,J)))
0------------------------------------------------------------------------
0INPUT DATA:  UIJ(X-RAY)
              UIJ(NEUTRON)
0ATOM       U11       U22       U33       U12       U13       U23

 C1    0.004860  0.003970  0.002160 -0.000670 -0.000890  0.000490
       0.004000  0.003960  0.003320 -0.000370  0.000320  0.001210
 C2    0.004330  0.004590  0.002320 -0.000450 -0.000850  0.000520
       0.003380  0.004600  0.003340 -0.000110  0.000230  0.000780
 C3    0.005880  0.003210  0.002160  0.000330 -0.000390  0.000320
       0.005000  0.003890  0.002960  0.000410  0.000580  0.000840
 C4    0.005860  0.003240  0.002140  0.000330 -0.000450  0.000430
       0.004780  0.003690  0.002910  0.000280  0.000260  0.000770
 K1    0.006020  0.004700  0.005330 -0.001100  0.000050  0.000130
       0.005100  0.004360  0.003980 -0.000340  0.000920  0.000600
 O1    0.006040  0.005800  0.003880 -0.002240 -0.001030  0.000810
       0.004740  0.006400  0.004490 -0.001890  0.000440  0.001410
 O2    0.006060  0.007510  0.002670 -0.001600 -0.001150  0.001960
       0.004770  0.007720  0.003810 -0.000740  0.000080  0.002090
 O3    0.007290  0.006100  0.002540 -0.001920 -0.002040  0.001230
       0.005230  0.006740  0.003660 -0.001280 -0.000610  0.001390
 O4    0.005210  0.006770  0.004040 -0.001950 -0.001340  0.000670
       0.003970  0.007280  0.004700 -0.001160 -0.000190  0.001540
 O5    0.011230  0.004420  0.001920  0.001060 -0.001020 -0.000110
       0.010130  0.004860  0.002810  0.000800  0.000110  0.000370
 O6    0.009590  0.003180  0.003720  0.000250 -0.000440  0.000180
       0.008500  0.003870  0.004550  0.000200  0.001090  0.000990
 O7    0.009600  0.005030  0.002040 -0.000500 -0.001160  0.000190
       0.008410  0.005370  0.003280 -0.000060  0.000020  0.000900
 O8    0.011420  0.003220  0.003810  0.000390 -0.000620  0.000400
       0.010700  0.003640  0.004450  0.000350  0.001160  0.001280
 O9    0.007590  0.005350  0.003430  0.001140 -0.000480  0.000530
       0.006720  0.006460  0.004330  0.001050  0.000470  0.001100
 O10   0.005670  0.007530  0.003950 -0.001500 -0.001280  0.001480
       0.005650  0.007510  0.004920 -0.000230  0.000680  0.001930
0MEAN VALUE OF 0.5*(UII(X-RAY) + UII(NEUTRON)) =   0.005070
 ESD FROM THE MEAN                             =   0.002067
0------------------------------------------------------------------------
0INPUT DATA:  SIGMA(UIJ(X-RAY))
              SIGMA(UIJ(NEUTRON))
0ATOM    SIGU11    SIGU22    SIGU33    SIGU12    SIGU13    SIGU23

 C1    0.000120  0.000110  0.000100  0.000100  0.000080  0.000080
       0.000120  0.000110  0.000100  0.000100  0.000080  0.000080
 C2    0.000120  0.000110  0.000100  0.000100  0.000080  0.000080
       0.000120  0.000110  0.000100  0.000100  0.000080  0.000080
 C3    0.000120  0.000110  0.000100  0.000100  0.000080  0.000080
       0.000120  0.000110  0.000100  0.000100  0.000080  0.000080
 C4    0.000120  0.000110  0.000100  0.000100  0.000090  0.000080
       0.000120  0.000110  0.000100  0.000100  0.000090  0.000080
 K1    0.000030  0.000030  0.000020  0.000020  0.000020  0.000020
       0.000030  0.000030  0.000030  0.000020  0.000020  0.000020
 O1    0.000110  0.000100  0.000090  0.000090  0.000070  0.000070
       0.000100  0.000100  0.000090  0.000090  0.000070  0.000080
 O2    0.000110  0.000110  0.000080  0.000090  0.000070  0.000080
       0.000100  0.000110  0.000080  0.000090  0.000070  0.000080
 O3    0.000110  0.000100  0.000080  0.000090  0.000070  0.000070
       0.000110  0.000100  0.000080  0.000090  0.000070  0.000070
 O4    0.000100  0.000100  0.000090  0.000090  0.000070  0.000080
       0.000100  0.000100  0.000090  0.000090  0.000070  0.000080
 O5    0.000130  0.000100  0.000080  0.000090  0.000080  0.000070
       0.000120  0.000100  0.000080  0.000090  0.000080  0.000070
 O6    0.000120  0.000090  0.000090  0.000090  0.000080  0.000070
       0.000120  0.000090  0.000090  0.000090  0.000080  0.000070
 O7    0.000120  0.000100  0.000080  0.000090  0.000080  0.000070
       0.000120  0.000100  0.000080  0.000090  0.000080  0.000070
 O8    0.000130  0.000090  0.000090  0.000090  0.000080  0.000070
       0.000120  0.000090  0.000090  0.000090  0.000080  0.000070
 O9    0.000110  0.000100  0.000090  0.000090  0.000080  0.000070
       0.000110  0.000100  0.000090  0.000090  0.000080  0.000070
 O10   0.000110  0.000110  0.000090  0.000090  0.000080  0.000080
       0.000100  0.000110  0.000090  0.000090  0.000080  0.000080
0------------------------------------------------------------------------
0SIGMA VALUES FOR LEAST-SQUARES WEIGHTS, WIJ = 1/SIGMAIJ**2
0SIGMAIJ = SQRT(SIGMA(UIJ(X-RAY))**2 + SIGMA(UIJ(NEUTRON))**2)
0ATOM   SIGMA11   SIGMA22   SIGMA33   SIGMA12   SIGMA13   SIGMA23

 C1    0.000170  0.000156  0.000141  0.000141  0.000113  0.000113
```

```
 C2    0.000170  0.000156  0.000141  0.000141  0.000113  0.000113
 C3    0.000170  0.000156  0.000141  0.000141  0.000113  0.000113
 C4    0.000170  0.000156  0.000141  0.000141  0.000127  0.000113
 K1    0.000042  0.000042  0.000036  0.000028  0.000028  0.000028
 O1    0.000149  0.000141  0.000127  0.000127  0.000099  0.000106
 O2    0.000149  0.000156  0.000113  0.000127  0.000099  0.000113
 O3    0.000156  0.000141  0.000113  0.000127  0.000099  0.000099
 O4    0.000141  0.000141  0.000127  0.000127  0.000099  0.000113
 O5    0.000177  0.000141  0.000113  0.000127  0.000113  0.000099
 O6    0.000170  0.000127  0.000127  0.000127  0.000113  0.000099
 O7    0.000170  0.000141  0.000113  0.000127  0.000113  0.000099
 O8    0.000177  0.000127  0.000127  0.000127  0.000113  0.000099
 O9    0.000156  0.000141  0.000127  0.000127  0.000113  0.000099
 O10   0.000149  0.000156  0.000127  0.000127  0.000113  0.000113
0------------------------------------------------------------------------
1PROGRAM UIJXN.  13:28:40  8-May-08.        OxHy2 XR/N/XResd/Nesd
0LEAST-SQUARES COMPARISON OF X-RAY AND NEUTRON THERMAL PARAMETERS
0ATOMIC DEBYE-WALLER FACTORS
0EXP(-M) = EXP(-2*PI**2*(SUM(I=1,3) SUM(J=1,3)
                          H(I)*H(J)*ASTAR(I)*ASTAR(J)*U(I,J)))
0------------------------------------------------------------------------
0RATIOS (UIJ(X-RAY)/UIJ(NEUTRON))
0ATOM       U11       U22       U33       U12       U13       U23

 C1       1.215     1.003     0.651     1.811    -2.781     0.405
 C2       1.281     0.998     0.695     4.091    -3.696     0.667
 C3       1.176     0.825     0.730     0.805    -0.672     0.381
 C4       1.226     0.878     0.735     1.179    -1.731     0.558
 K1       1.180     1.078     1.339     3.235     0.054     0.217
 O1       1.274     0.906     0.864     1.185    -2.341     0.574
 O2       1.270     0.973     0.701     2.162   -14.375     0.938
 O3       1.394     0.905     0.694     1.500     3.344     0.885
 O4       1.312     0.930     0.860     1.681     7.053     0.435
 O5       1.109     0.909     0.683     1.325    -9.273    -0.297
 O6       1.128     0.822     0.818     1.250    -0.404     0.182
 O7       1.141     0.937     0.622     8.333   -58.000     0.211
 O8       1.067     0.885     0.856     1.114    -0.534     0.313
 O9       1.129     0.828     0.792     1.086    -1.021     0.482
 O10      1.004     1.003     0.803     6.522    -1.882     0.767
0MEAN RATIO OF UII VALUES, <UII(X-RAY)/UII(NEUTRON)> =      0.970
 ESD FROM THE MEAN                                  =      0.208
0------------------------------------------------------------------------
0DIFFERENCES (UIJ(X-RAY) - UIJ(NEUTRON))
0ATOM       U11       U22       U33       U12       U13       U23

 C1    0.000860  0.000010 -0.001160 -0.000300 -0.001210 -0.000720
 C2    0.000950 -0.000010 -0.001020 -0.000340 -0.001080 -0.000260
 C3    0.000880 -0.000680 -0.000800 -0.000080 -0.000970 -0.000520
 C4    0.001080 -0.000450 -0.000770  0.000050 -0.000710 -0.000340
 K1    0.000920  0.000340  0.001350 -0.000760 -0.000870 -0.000470
 O1    0.001300 -0.000600 -0.000610 -0.000350 -0.001470 -0.000600
 O2    0.001290 -0.000210 -0.001140 -0.000860 -0.001230 -0.000130
 O3    0.002060 -0.000640 -0.001120 -0.000640 -0.001430 -0.000160
 O4    0.001240 -0.000510 -0.000660 -0.000790 -0.001150 -0.000870
 O5    0.001100 -0.000440 -0.000890  0.000260 -0.001130 -0.000480
 O6    0.001090 -0.000690 -0.000830  0.000050 -0.001530 -0.000810
 O7    0.001190 -0.000340 -0.001240 -0.000440 -0.001180 -0.000710
 O8    0.000720 -0.000420 -0.000640  0.000040 -0.001780 -0.000880
 O9    0.000870 -0.001110 -0.000900  0.000090 -0.000950 -0.000570
 O10   0.000020  0.000020 -0.000970 -0.001270 -0.001960 -0.000450
0MEAN ABSOLUTE DELTA    =   0.000768
 ESD FROM THE MEAN      =   0.000451
0ROOT-MEAN-SQUARE DELTA =   0.000889
 ROOT-MEAN-SQUARE DELTA/SIGMA(DELTA) =   9.60
0------------------------------------------------------------------------
1PROGRAM UIJXN.  13:28:40  8-May-08.        OxHy2 XR/N/XResd/Nesd
0LEAST-SQUARES COMPARISON OF X-RAY AND NEUTRON THERMAL PARAMETERS
0ATOMIC DEBYE-WALLER FACTORS
0EXP(-M) = EXP(-2*PI**2*(SUM(I=1,3) SUM(J=1,3)
                          H(I)*H(J)*ASTAR(I)*ASTAR(J)*U(I,J)))
0------------------------------------------------------------------------
01.  ISOTROPIC TEMPERATURE CORRECTION FACTOR
 ------------------------------------------
0UX(I,J) = FACTOR*UN(I,J)
0CHISQ = SUM(W(A,I,J)*(UX(A,I,J) - FACTOR*UN(A,I,J))**2)
 Z     = SQRT(CHISQ/(NOBS - NPAR)
 RMSD  = SQRT(CHISQ/SUMW)
0FROM UII'S ONLY
 ---------------
0FACTOR
  1.066
0Z    =  0.8554E+01
 NOBS = 45
 NPAR =  1
0RMSD =  0.000899932
0FROM UII'S AND UIJ'S
 --------------------
```

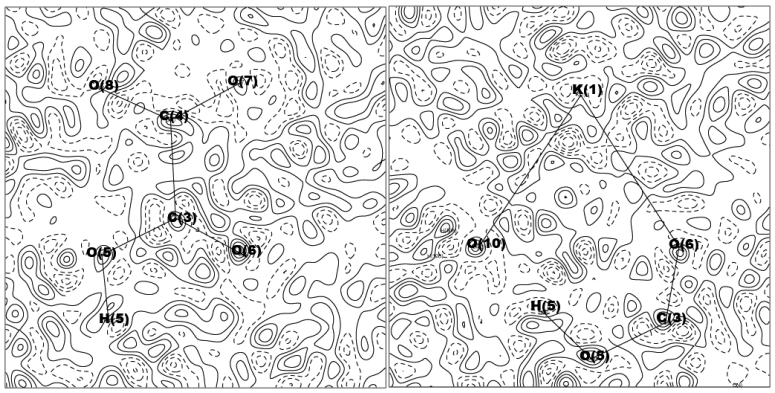
```
0FACTOR
  1.042
0Z    =  0.9522E+01
 NOBS = 90
 NPAR =  1
0RMSD =  0.000857911
0------------------------------------------------------------------------
1PROGRAM UIJXN.  13:28:40  8-May-08.        OxHy2 XR/N/XResd/Nesd
0LEAST-SQUARES COMPARISON OF X-RAY AND NEUTRON THERMAL PARAMETERS
0ATOMIC DEBYE-WALLER FACTORS
0EXP(-M) = EXP(-2*PI**2*(SUM(I=1,3) SUM(J=1,3)
                          H(I)*H(J)*ASTAR(I)*ASTAR(J)*U(I,J)))
0------------------------------------------------------------------------
02.   ANISOTROPIC TENSOR CORRECTION FOR ABSORPTION, EXTINCTION, TDS, OR MULTIPLE-REFLECTION DIFFRACTION
EFFECTS
 ------------------------------------------------------------------------------------------------------------------
---
0UX(I,J) = UN(I,J) + DELTA(I,J)
0CHISQ = SUM(W(A,I,J)*(UX(A,I,J) - UN(A,I,J) - DELTA(I,J))**2)
0  DELTA(1,1)  DELTA(2,2)  DELTA(3,3)  DELTA(1,2)  DELTA(1,3)   DELTA(2,3)
     0.000986   -0.000095    0.000135   -0.000592   -0.001069   -0.000507
0Z    =  0.6026E+01
 NOBS = 90
 NPAR =  6
0RMSD =  0.000527516
0------------------------------------------------------------------------
03.  SUM OF ISOTROPIC TEMPERATURE CORRECTION AND ANISOTROPIC DIFFRACTION CORRECTIONS
 ---------------------------------------------------------------------------
0UX(I,J) = FACTOR*UN(I,J) + DELTA(I,J)
0CHISQ = SUM(W(A,I,J)*(UX(A,I,J) - FACTOR*UN(A,I,J) - DELTA(I,J))**2
0      FACTOR
        1.029
0    SIGMA(F)
        0.076
0  DELTA(1,1)  DELTA(2,2)  DELTA(3,3)  DELTA(1,2)  DELTA(1,3)  DELTA(2,3)
     0.000823   -0.000239    0.000021   -0.000584   -0.001088   -0.000533
0  SIGMA(1,1)  SIGMA(2,2)  SIGMA(3,3)  SIGMA(1,2)  SIGMA(1,3)  SIGMA(2,3)
     0.000456    0.000410    0.000330    0.000135    0.000132    0.000138
0Z    =  0.6057E+01
 NOBS = 90
 NPAR =  7
0RMSD =  0.000527036
0------------------------------------------------------------------------
1PROGRAM UIJXN.  13:28:40  8-May-08.        OxHy2 XR/N/XResd/Nesd
0LEAST-SQUARES COMPARISON OF X-RAY AND NEUTRON THERMAL PARAMETERS
0ATOMIC DEBYE-WALLER FACTORS
0EXP(-M) = EXP(-2*PI**2*(SUM(I=1,3) SUM(J=1,3)
                          H(I)*H(J)*ASTAR(I)*ASTAR(J)*U(I,J)))
0------------------------------------------------------------------------
04.  ANISOTROPIC SCALING FACTORS
 -------------------------------
0UX(I,J) = FACTOR(I,J)*UN(I,J)
0CHISQ = SUM(W(A,I,J)*UX(A,I,J) - FACTOR(I,J)*UN(A,I,J))**2)
0 FACTOR(1,1) FACTOR(2,2) FACTOR(3,3) FACTOR(1,2) FACTOR(1,3) FACTOR(2,3)
        1.164       0.974       1.042       1.769      -0.069       0.529
0FROM UII'S ONLY
 ---------------
0Z    =  0.7853E+01
 NOBS = 45
 NPAR =  3
0RMSD =  0.000486045
0FROM UII'S AND UIJ'S
 --------------------
0Z    =  0.7466E+01
 NOBS = 90
 NPAR =  6
0RMSD =  0.000653525
0------------------------------------------------------------------------
```

Output from XDFFT for D3(AU) final model using all data in the summation

Function values range from -0.507 to 0.414. RMS = 0.099

	PK(1)	is 0.75 A from K(1)	0.0635	0.0793	0.2786	0.41
	PK(2)	is 1.58 A from K(1)	0.2452	0.2818	0.4058	0.40
	PK(3)	is 0.57 A from O(4)	-0.2573	0.1090	0.1262	0.37
23	PK(4)	.....	0.7832	0.2819	0.9639	0.36
24	PK(5)	.....	0.9368	0.4685	0.9243	0.35
	PK(6)	is 0.61 A from C(2)	-0.3763	-0.0562	0.0520	0.34
	PK(7)	is 1.25 A from K(1)	0.2851	0.3034	0.2589	0.34
	PK(8)	is 2.26 A from K(1)	0.1503	0.1416	0.4848	0.34
25	PK(9)	.....	0.6277	0.3872	0.8534	0.34
26	PK(10)	.....	0.7805	0.1397	0.3885	0.34
	HL(1)	is 0.75 A from K(1)	0.2510	0.1055	0.2411	-0.51
	HL(2)	is 0.78 A from K(1)	0.0937	0.1938	0.3140	-0.45
27	HL(3)	.....	0.5017	0.4465	0.8166	-0.42
	HL(4)	is 0.49 A from O(4)	-0.2847	0.0636	0.0911	-0.41
	HL(5)	is 0.37 A from O(9)	-0.1575	-0.0275	0.3531	-0.39
	HL(6)	is 0.88 A from K(1)	0.0424	0.0807	0.2255	-0.37
	HL(7)	is 0.36 A from O(6)	0.2850	-0.1404	0.4633	-0.37
28	HL(8)	.....	0.4672	0.1701	0.8373	-0.36
29	HL(9)	.....	0.1187	0.3048	0.4812	-0.34
30	HL(10)	.....	0.3076	0.3320	0.5386	-0.34

Residual density maps using all data



Charge density parameters

Label	Pv	P11	P1-1	P10	P20	P21	P2-1	P22	P2-2	P30	P31	P3-1	P32	P3-2	P33	P3-3	k	k'
K(1)	18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1
O(1)	6.383(17)	-0.034(10)	0.010(8)	0.004(8)	-0.093(9)	-0.005(8)	0.001(8)	-0.065(9)	0.025(8)	-0.017(8)	-0.016(8)	0.001(7)	-0.009(7)	0.008(7)	0.041(7)	-0.006(7)	0.9723(10)	0.956(23)
O(2)	6.426(19)	0.020(9)	-0.039(9)	0.002(9)	-0.013(9)	-0.001(9)	-0.012(8)	0.089(9)	-0.008(9)	-0.007(8)	-0.031(8)	-0.026(8)	-0.010(8)	-0.006(7)	0.088(7)	-0.021(8)	0.9742(12)	0.957(28)
O(3)	6.371(19)	0.014(9)	-0.062(9)	0.007(9)	-0.037(9)	-0.009(9)	-0.005(8)	0.063(8)	-0.009(9)	0.009(8)	-0.029(8)	-0.014(8)	-0.003(7)	0.003(7)	0.095(7)	-0.009(7)	0.9742(12)	0.957(28)
O(4)	6.348(17)	-0.045(10)	-0.002(8)	0.004(8)	-0.083(9)	0.011(8)	-0.007(8)	-0.067(9)	-0.029(8)	-0.005(8)	-0.004(8)	-0.001(8)	-0.001(7)	0.006(7)	0.054(7)	-0.002(7)	0.9723(10)	0.956(23)
O(5)	6.40(2)	-0.011(9)	-0.033(9)	0.003(9)	-0.052(9)	-0.014(9)	-0.011(9)	0.048(9)	-0.004(9)	-0.001(8)	-0.023(8)	-0.017(8)	-0.009(8)	0.007(8)	0.100(8)	-0.020(8)	0.9742(12)	0.957(28)
O(6)	6.387(17)	-0.049(9)	-0.005(8)	-0.006(8)	-0.102(9)	0.032(9)	-0.011(8)	-0.064(8)	0.006(8)	-0.005(8)	-0.002(8)	-0.019(7)	0.007(8)	-0.008(7)	0.047(7)	-0.003(7)	0.9723(10)	0.956(23)
O(7)	6.423(17)	-0.042(9)	-0.012(8)	-0.009(8)	-0.079(9)	-0.002(9)	-0.022(8)	-0.031(9)	-0.040(8)	0.002(8)	-0.013(8)	0.001(7)	-0.013(8)	-0.002(7)	0.071(7)	-0.012(7)	0.9723(10)	0.956(23)
O(8)	6.403(16)	-0.045(9)	-0.012(8)	-0.004(8)	-0.107(9)	-0.048(9)	0.016(8)	-0.078(8)	0.005(8)	0.006(8)	-0.028(8)	-0.006(7)	-0.002(8)	0.008(7)	0.043(7)	-0.004(7)	0.9723(10)	0.956(23)
O(9)	6.55(3)	-0.029(8)	-0.028(8)	0.002(8)	0.001(9)	-0.038(8)	-0.017(8)	-0.017(7)	0.016(8)	-0.002(8)	-0.034(7)	-0.054(7)	-0.007(7)	0.016(7)	0.093(7)	-0.037(7)	0.9645(16)	0.967(26)
O(10)	6.55(3)	-0.027(8)	-0.031(8)	0.007(8)	0.013(9)	-0.001(8)	0.012(8)	-0.021(7)	0.043(8)	0.006(8)	-0.033(7)	-0.043(8)	0.008(7)	-0.016(7)	0.109(7)	-0.040(7)	0.9645(16)	0.967(26)
C(1)	3.83(2)	0.043(11)	-0.018(9)	-0.006(9)	-0.237(10)	-0.003(9)	-0.006(9)	0.007(11)	-0.017(9)	0.008(12)	0.036(11)	-0.003(10)	-0.002(10)	0.014(11)	0.302(11)	0.010(13)	1.013(2)	1.002(9)
C(2)	3.80(2)	0.054(11)	-0.008(9)	0.002(9)	-0.257(10)	0.007(9)	-0.003(9)	0.027(11)	0.004(9)	0.007(12)	0.003(11)	0.010(10)	-0.009(10)	0.028(11)	0.309(11)	0.018(14)	1.013(2)	1.002(9)
C(3)	3.79(2)	0.078(11)	-0.044(10)	0.021(9)	-0.265(10)	0.016(9)	0.001(9)	0.031(10)	0.015(10)	-0.014(11)	-0.007(11)	0.012(10)	0.003(11)	0.008(11)	0.294(12)	-0.001(12)	1.013(2)	1.002(9)
C(4)	3.82(2)	0.032(11)	0.017(10)	-0.007(8)	-0.245(10)	-0.030(9)	0.004(9)	0.014(10)	-0.036(10)	0.021(11)	-0.002(11)	-0.003(10)	-0.011(11)	-0.012(11)	0.293(12)	0.034(12)	1.013(2)	1.002(9)
H(2)	0.579(13)	0.001(8)	-0.004(8)	0.057(11)	0.037(16)	0.018(14)	-0.042(14)	-0.010(12)	0.003(12)	0	0	0	0	0	0	0	1.2	1.2
H(3)	0.593(12)	-0.016(9)	0.001(8)	0.023(10)	0.089(16)	0.015(14)	0.043(14)	0.017(12)	-0.001(12)	0	0	0	0	0	0	0	1.2	1.2
H(5)	0.600(13)	0.017(8)	-0.003(9)	0.101(11)	0.071(16)	0.037(13)	-0.011(14)	-0.014(12)	0.013(11)	0	0	0	0	0	0	0	1.2	1.2
H(9A)	0.689(9)	0	0	0.110(7)	0.069(8)	0	0	0	0	0	0	0	0	0	0	0	1.2	1.2
H(9B)	0.689(9)	0	0	0.110(7)	0.069(8)	0	0	0	0	0	0	0	0	0	0	0	1.2	1.2
H(10A)	0.689(9)	0	0	0.110(7)	0.069(8)	0	0	0	0	0	0	0	0	0	0	0	1.2	1.2
H(10B)	0.689(9)	0	0	0.110(7)	0.069(8)	0	0	0	0	0	0	0	0	0	0	0	1.2	1.2