Crystallographic Information File (CIF)

```
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#-----------------------  COMPOUND 9a  ---------------------------------
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_computing_cell_refinement       'Rigaku/MSC diffractometer control'
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
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O2 O 0.1227(4) 0.19061(6) 0.9653(3) 0.0815(7) Uani 1 d . . .
O3 O 0.2944(4) 0.21646(5) 0.7625(3) 0.0761(6) Uani 1 d . . .
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C2 C 0.2010(4) 0.03721(6) 0.8395(3) 0.0373(5) Uani 1 d . . .
H2 H 0.2807 0.0300 0.9665 0.045 Uiso 1 calc R . .
C3 C 0.2031(4) 0.08565(6) 0.8116(3) 0.0338(5) Uani 1 d . . .
C4 C 0.2608(3) 0.08994(6) 0.6353(3) 0.0334(5) Uani 1 d . . .
C5 C 0.3508(4) 0.05474(7) 0.5890(3) 0.0413(5) Uani 1 d . . .
H5 H 0.4117 0.0521 0.4921 0.050 Uiso 1 calc R . .
C6 C -0.0401(4) 0.01703(7) 0.7789(4) 0.0539(7) Uani 1 d . . .
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H6B H -0.1303 0.0276 0.8530 0.081 Uiso 1 calc R . .
H6C H -0.0258 -0.0133 0.7917 0.081 Uiso 1 calc R . .
C7 C 0.3924(4) 0.10675(7) 0.9690(3) 0.0453(6) Uani 1 d . . .
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H7B H 0.5332 0.0899 0.9952 0.054 Uiso 1 calc R . .
C8 C 0.4463(5) 0.15231(7) 0.9267(3) 0.0556(7) Uani 1 d . . .
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H8B H 0.5470 0.1517 0.8497 0.067 Uiso 1 calc R . .
C9 C 0.2313(5) 0.17780(7) 0.8331(3) 0.0541(7) Uani 1 d . . .
C10 C 0.0592(4) 0.15198(7) 0.6824(3) 0.0452(6) Uani 1 d . . .
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H11B H -0.1493 0.0990 0.6918 0.056 Uiso 1 calc R . .
C12 C 0.1624(4) 0.13113(7) 0.5391(3) 0.0422(6) Uani 1 d . . .
C13 C 0.3359(5) 0.15733(8) 0.4728(4) 0.0634(8) Uani 1 d . . .
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H13B H 0.2605 0.1824 0.4114 0.095 Uiso 1 calc R . .
H13C H 0.3913 0.1405 0.3904 0.095 Uiso 1 calc R . .
C14 C -0.0380(5) 0.11880(8) 0.3683(3) 0.0651(8) Uani 1 d . . .
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H14B H -0.1107 0.1441 0.3077 0.098 Uiso 1 calc R . .
H14C H -0.1502 0.1021 0.4037 0.098 Uiso 1 calc R . .
C15 C 0.0364(8) 0.23152(10) 0.9246(6) 0.1047(13) Uani 1 d . . .
H15A H 0.0494 0.2476 1.0346 0.126 Uiso 1 calc R . .
H15B H -0.1249 0.2309 0.8509 0.126 Uiso 1 calc R . .
C16 C 0.1855(8) 0.25013(10) 0.8219(6) 0.1173(16) Uani 1 d . . .
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O3 0.1065(16) 0.0297(9) 0.0880(14) -0.0001(9) 0.0232(12) -0.0054(10)
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C2 0.0403(13) 0.0347(11) 0.0336(11) 0.0030(9) 0.0063(10) -0.0018(9)
C3 0.0365(12) 0.0321(11) 0.0322(11) -0.0002(9) 0.0092(9) -0.0005(9)
C4 0.0332(11) 0.0343(11) 0.0314(11) -0.0011(8) 0.0077(9) -0.0045(9)
C5 0.0458(13) 0.0441(13) 0.0378(12) -0.0026(10) 0.0183(11) -0.0002(10)
C6 0.0526(16) 0.0475(14) 0.0625(16) 0.0029(12) 0.0189(13) -0.0104(12)
C7 0.0527(14) 0.0402(12) 0.0371(12) -0.0053(9) 0.0047(11) 0.0031(10)
C8 0.0612(17) 0.0396(13) 0.0524(14) -0.0089(11) -0.0034(12) -0.0023(12)
C9 0.0733(18) 0.0336(12) 0.0555(16) -0.0032(11) 0.0195(14) 0.0061(12)
C10 0.0410(13) 0.0379(12) 0.0535(14) 0.0061(10) 0.0090(11) 0.0111(10)
C11 0.0421(13) 0.0473(13) 0.0530(14) 0.0037(11) 0.0179(11) 0.0069(11)
C12 0.0503(14) 0.0355(12) 0.0387(12) 0.0037(9) 0.0104(10) -0.0018(10)
C13 0.080(2) 0.0524(15) 0.0622(17) 0.0100(13) 0.0287(15) -0.0088(14)
C14 0.076(2) 0.0574(16) 0.0448(14) 0.0067(12) -0.0082(14) 0.0011(14)
C15 0.144(4) 0.058(2) 0.110(3) -0.0116(19) 0.035(3) 0.041(2)
C16 0.181(5) 0.0385(18) 0.131(4) 0.001(2) 0.046(3) 0.018(2)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
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 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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O3 C9 1.429(3) . ?
C1 C5 1.471(3) . ?
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C2 C6 1.527(3) . ?
C2 C3 1.538(3) . ?
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C7 C8 1.525(3) . ?
C8 C9 1.512(3) . ?
C9 C10 1.538(3) . ?
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C15 C16 1.486(6) . ?

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C5 C1 C2 108.22(18) . . ?
C6 C2 C1 108.28(17) . . ?
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C4 C3 C2 103.21(16) . . ?
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C4 C12 C10 101.06(16) . . ?
C13 C12 C10 117.81(19) . . ?
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#---------------------- COMPOUND **9b** ----------------------------------
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 'C'  'C'   0.0033   0.0016
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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 Fine + weakly diffracting sample
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_diffrn_measurement_device_type 'Rigaku AFC7S'
_diffrn_measurement_method      '\w/\2q'
_diffrn_detector_area_resol_mean ?
_diffrn_standards_number        3
_diffrn_standards_interval_count 150
_diffrn_standards_interval_time ?
_diffrn_standards_decay_%       1.24
_diffrn_reflns_number           2138
_diffrn_reflns_av_R_equivalents 0.0295
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_diffrn_reflns_av_sigmaI/netI     0.0719
_diffrn_reflns_limit_h_min        0
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_diffrn_reflns_limit_k_min        0
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_diffrn_reflns_limit_l_min        -15
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_diffrn_reflns_theta_min          2.51
_diffrn_reflns_theta_max          23.00
_reflns_number_total              1932
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_reflns_threshold_expression      >2sigma(I)

_computing_data_collection        'Rigaku/MSC diffractometer control'
_computing_cell_refinement        'Rigaku/MSC diffractometer control'
_computing_data_reduction         'teXsan'
_computing_structure_solution     'SIR'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   'SHELXL-97 (Sheldrick, 1997)'

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

_refine_ls_structure_factor_coef  Fsqd
_refine_ls_matrix_type            full
_refine_ls_weighting_scheme
 'calc w=1/[\s^2^(Fo^2^)+(0.0816P)^2^+1.7548P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     calc
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_refine_ls_extinction_coef 0.010(3)
_refine_ls_extinction_expression
'Fc^*^=kFc[1+0.001xFc^2^\l^3^/sin(2\q)]^-1/4^'
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_refine_ls_number_parameters 176
_refine_ls_number_restraints 0
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_atom_site_refinement_flags
_atom_site_disorder_assembly
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O2 O 0.7445(5) 0.16139(16) 0.67355(19) 0.0353(8) Uani 1 d . . .
O3 O 0.5606(5) 0.11391(16) 0.5378(2) 0.0391(8) Uani 1 d . . .
C1 C 0.1417(7) 0.4497(2) 0.6405(3) 0.0286(10) Uani 1 d . . .
C2 C 0.1583(7) 0.4067(2) 0.5489(3) 0.0306(10) Uani 1 d . . .
H2 H 0.0729 0.4187 0.4919 0.037 Uiso 1 calc R . .
C3 C 0.3116(6) 0.3487(2) 0.5589(2) 0.0264(9) Uani 1 d . . .
C4 C 0.4066(7) 0.3399(2) 0.6606(3) 0.0260(9) Uani 1 d . . .
C5 C 0.3354(7) 0.4208(2) 0.7065(3) 0.0297(10) Uani 1 d . . .
H5 H 0.4579 0.4610 0.6988 0.036 Uiso 1 calc R . .
C6 C 0.2890(8) 0.4215(3) 0.8111(3) 0.0395(11) Uani 1 d . . .

H6A H 0.2383 0.4763 0.8289 0.059 Uiso 1 calc R . .
H6B H 0.4242 0.4077 0.8493 0.059 Uiso 1 calc R . .
H6C H 0.1744 0.3808 0.8228 0.059 Uiso 1 calc R . .
C7 C 0.3189(7) 0.2633(2) 0.7091(3) 0.0280(9) Uani 1 d . . .
H7A H 0.3962 0.2573 0.7726 0.034 Uiso 1 calc R . .
H7B H 0.1598 0.2709 0.7185 0.034 Uiso 1 calc R . .
C8 C 0.3493(7) 0.1843(2) 0.6524(3) 0.0311(10) Uani 1 d . . .
H8A H 0.3390 0.1366 0.6956 0.037 Uiso 1 calc R . .
H8B H 0.2275 0.1798 0.6028 0.037 Uiso 1 calc R . .
C9 C 0.5657(6) 0.1804(2) 0.6059(3) 0.0267(9) Uani 1 d . . .
C10 C 0.6307(7) 0.2622(2) 0.5600(3) 0.0278(9) Uani 1 d . . .
H10 H 0.7729 0.2566 0.5281 0.033 Uiso 1 calc R . .
C11 C 0.6517(6) 0.3259(2) 0.6417(3) 0.0275(9) Uani 1 d . . .
H11A H 0.7352 0.3034 0.6984 0.033 Uiso 1 calc R . .
H11B H 0.7231 0.3772 0.6215 0.033 Uiso 1 calc R . .
C12 C 0.4465(7) 0.3011(2) 0.4908(3) 0.0317(10) Uani 1 d . . .
C13 C 0.5564(8) 0.3647(3) 0.4272(3) 0.0440(12) Uani 1 d . . .
H13A H 0.4420 0.3960 0.3908 0.066 Uiso 1 calc R . .
H13B H 0.6494 0.3361 0.3832 0.066 Uiso 1 calc R . .
H13C H 0.6475 0.4024 0.4671 0.066 Uiso 1 calc R . .
C14 C 0.3101(8) 0.2429(3) 0.4240(3) 0.0407(12) Uani 1 d . . .
H14A H 0.2355 0.2020 0.4619 0.061 Uiso 1 calc R . .
H14B H 0.4082 0.2149 0.3817 0.061 Uiso 1 calc R . .
H14C H 0.1998 0.2748 0.3861 0.061 Uiso 1 calc R . .
C15 C 0.7897(7) 0.0755(2) 0.6653(3) 0.0330(10) Uani 1 d . . .
H15A H 0.6909 0.0422 0.7035 0.040 Uiso 1 calc R . .
H15B H 0.9451 0.0628 0.6853 0.040 Uiso 1 calc R . .
C16 C 0.7439(7) 0.0610(3) 0.5610(3) 0.0366(10) Uani 1 d . . .
H16A H 0.8727 0.0761 0.5248 0.044 Uiso 1 calc R . .
H16B H 0.7052 0.0027 0.5480 0.044 Uiso 1 calc R . .

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 _atom_site_aniso_U_11
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 _atom_site_aniso_U_33
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 _atom_site_aniso_U_13
 _atom_site_aniso_U_12
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O2 0.0433(17) 0.0295(15) 0.0310(15) -0.0002(12) -0.0145(13) 0.0072(13)
O3 0.0503(19) 0.0276(15) 0.0373(16) -0.0072(13) -0.0163(13) 0.0069(13)
C1 0.038(2) 0.0179(19) 0.029(2) 0.0020(16) -0.0042(18) -0.0001(19)
C2 0.037(2) 0.026(2) 0.027(2) 0.0036(16) -0.0116(17) -0.0010(19)
C3 0.036(2) 0.0218(19) 0.020(2) 0.0026(16) -0.0074(17) -0.0068(18)
C4 0.035(2) 0.023(2) 0.0193(19) 0.0004(15) -0.0066(16) -0.0036(17)
C5 0.040(2) 0.023(2) 0.025(2) -0.0017(16) -0.0052(17) -0.0046(18)
C6 0.060(3) 0.028(2) 0.030(2) -0.0016(18) -0.006(2) 0.001(2)
C7 0.032(2) 0.027(2) 0.0237(19) 0.0036(16) -0.0033(16) -0.0037(17)
C8 0.038(2) 0.024(2) 0.031(2) 0.0066(17) -0.0042(18) -0.0045(18)
C9 0.029(2) 0.026(2) 0.024(2) -0.0023(16) -0.0075(16) 0.0048(17)
C10 0.026(2) 0.031(2) 0.026(2) -0.0022(16) -0.0020(16) 0.0049(18)
C11 0.029(2) 0.027(2) 0.025(2) 0.0020(16) -0.0066(16) -0.0021(17)
C12 0.045(3) 0.023(2) 0.025(2) -0.0011(16) -0.0137(18) 0.0055(18)
C13 0.067(3) 0.037(3) 0.028(2) 0.0074(19) 0.000(2) 0.010(2)
C14 0.052(3) 0.041(3) 0.026(2) -0.0099(19) -0.017(2) 0.010(2)
C15 0.040(2) 0.026(2) 0.033(2) 0.0081(17) -0.0014(18) 0.0077(18)
C16 0.039(2) 0.030(2) 0.040(2) 0.0001(19) -0.0013(19) 0.010(2)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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_geom_bond_site_symmetry_2
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O2 C15 1.429(5) . ?
O2 C9 1.435(4) . ?
O3 C16 1.429(5) . ?
O3 C9 1.444(4) . ?

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C1 C2 1.476(6) . ?
C1 C5 1.529(5) . ?
C2 C3 1.326(5) . ?
C3 C12 1.510(6) . ?
C3 C4 1.519(5) . ?
C4 C7 1.532(5) . ?
C4 C5 1.538(5) . ?
C4 C11 1.543(6) . ?
C5 C6 1.517(6) . ?
C7 C8 1.528(5) . ?
C8 C9 1.504(6) . ?
C9 C10 1.540(5) . ?
C10 C11 1.548(5) . ?
C10 C12 1.572(5) . ?
C12 C14 1.540(5) . ?
C12 C13 1.545(6) . ?
C15 C16 1.498(6) . ?

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C15 O2 C9 107.3(3) . . ?
C16 O3 C9 108.3(3) . . ?
O1 C1 C2 127.6(3) . . ?
O1 C1 C5 124.9(3) . . ?
C2 C1 C5 107.2(3) . . ?
C3 C2 C1 109.1(3) . . ?
C2 C3 C12 134.4(3) . . ?
C2 C3 C4 113.0(3) . . ?
C12 C3 C4 111.2(3) . . ?
C3 C4 C7 112.0(3) . . ?
C3 C4 C5 102.5(3) . . ?
C7 C4 C5 113.2(3) . . ?
C3 C4 C11 99.6(3) . . ?
C7 C4 C11 108.7(3) . . ?
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C5 C4 C11 119.8(3) . . ?
C6 C5 C1 114.1(4) . . ?
C6 C5 C4 119.2(3) . . ?
C1 C5 C4 103.4(3) . . ?
C8 C7 C4 113.2(3) . . ?
C9 C8 C7 113.5(3) . . ?
O2 C9 O3 105.4(3) . . ?
O2 C9 C8 111.4(3) . . ?
O3 C9 C8 109.7(3) . . ?
O2 C9 C10 105.2(3) . . ?
O3 C9 C10 111.3(3) . . ?
C8 C9 C10 113.5(3) . . ?
C9 C10 C11 106.1(3) . . ?
C9 C10 C12 114.7(3) . . ?
C11 C10 C12 102.5(3) . . ?
C4 C11 C10 100.9(3) . . ?
C3 C12 C14 114.2(4) . . ?
C3 C12 C13 107.2(3) . . ?
C14 C12 C13 106.9(3) . . ?
C3 C12 C10 101.8(3) . . ?
C14 C12 C10 117.9(3) . . ?
C13 C12 C10 108.3(3) . . ?
O2 C15 C16 102.0(3) . . ?
O3 C16 C15 103.1(3) . . ?

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O1 C1 C2 C3 -175.8(4) . . . . ?
C5 C1 C2 C3 9.8(4) . . . . ?
C1 C2 C3 C12 -160.4(4) . . . . ?
C1 C2 C3 C4 4.6(5) . . . . ?

C2 C3 C4 C7 104.9(4) . . . . ?
C12 C3 C4 C7 -86.5(4) . . . . ?
C2 C3 C4 C5 -16.7(4) . . . . ?
C12 C3 C4 C5 151.8(3) . . . . ?
C2 C3 C4 C11 -140.3(3) . . . . ?
C12 C3 C4 C11 28.3(4) . . . . ?
O1 C1 C5 C6 35.0(5) . . . . ?
C2 C1 C5 C6 -150.4(3) . . . . ?
O1 C1 C5 C4 166.0(4) . . . . ?
C2 C1 C5 C4 -19.5(4) . . . . ?
C3 C4 C5 C6 148.7(4) . . . . ?
C7 C4 C5 C6 27.9(5) . . . . ?
C11 C4 C5 C6 -102.4(4) . . . . ?
C3 C4 C5 C1 20.9(4) . . . . ?
C7 C4 C5 C1 -100.0(3) . . . . ?
C11 C4 C5 C1 129.7(3) . . . . ?
C3 C4 C7 C8 53.2(4) . . . . ?
C5 C4 C7 C8 168.4(3) . . . . ?
C11 C4 C7 C8 -55.9(4) . . . . ?
C4 C7 C8 C9 39.2(4) . . . . ?
C15 O2 C9 O3 -19.5(4) . . . . ?
C15 O2 C9 C8 99.4(4) . . . . ?
C15 O2 C9 C10 -137.2(3) . . . . ?
C16 O3 C9 O2 -4.7(4) . . . . ?
C16 O3 C9 C8 -124.7(3) . . . . ?
C16 O3 C9 C10 108.9(3) . . . . ?
C7 C8 C9 O2 76.3(4) . . . . ?
C7 C8 C9 O3 -167.4(3) . . . . ?
C7 C8 C9 C10 -42.2(4) . . . . ?
O2 C9 C10 C11 -61.1(4) . . . . ?
O3 C9 C10 C11 -174.7(3) . . . . ?
C8 C9 C10 C11 61.0(4) . . . . ?
O2 C9 C10 C12 -173.4(3) . . . . ?
O3 C9 C10 C12 73.0(4) . . . . ?
C8 C9 C10 C12 -51.4(4) . . . . ?
C3 C4 C11 C10 -45.4(3) . . . . ?
C7 C4 C11 C10 72.0(3) . . . . ?
C5 C4 C11 C10 -155.8(3) . . . . ?
C9 C10 C11 C4 -73.3(3) . . . . ?
C12 C10 C11 C4 47.2(4) . . . . ?

C2 C3 C12 C14 -66.2(6) . . . . ?
C4 C3 C12 C14 128.6(3) . . . . ?
C2 C3 C12 C13 52.1(6) . . . . ?
C4 C3 C12 C13 -113.2(3) . . . . ?
C2 C3 C12 C10 165.6(4) . . . . ?
C4 C3 C12 C10 0.4(4) . . . . ?
C9 C10 C12 C3 85.3(4) . . . . ?
C11 C10 C12 C3 -29.1(4) . . . . ?
C9 C10 C12 C14 -40.5(5) . . . . ?
C11 C10 C12 C14 -154.9(4) . . . . ?
C9 C10 C12 C13 -161.9(3) . . . . ?
C11 C10 C12 C13 83.6(4) . . . . ?
C9 O2 C15 C16 34.6(4) . . . . ?
C9 O3 C16 C15 25.4(4) . . . . ?
O2 C15 C16 O3 -36.3(4) . . . . ?

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_diffrn_reflns_theta_full 23.00
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#------------------------- COMPOUND **11** --------------------------------
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;
_chemical_name_common ?
_chemical_formula_moiety ?
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'C16 H24 O3'
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_atom_type_symbol
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_atom_type_scat_dispersion_imag
_atom_type_scat_source
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'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'C' 'C' 0.0033 0.0016
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
'H' 'H' 0.0000 0.0000
'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting monoclinic
_symmetry_space_group_name_H-M P21

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

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_cell_length_b 8.3930(3)
_cell_length_c 10.2120(4)
_cell_angle_alpha 90.00
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_cell_angle_gamma 90.00
_cell_volume 683.70(4)
_cell_formula_units_Z 2
_cell_measurement_temperature 150(2)
_cell_measurement_reflns_used 17654
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_exptl_special_details
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_diffrn_reflns_limit_k_max       10
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_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     ?
_computing_publication_material   'SHELXL-97 (Sheldrick, 1997)'

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

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_refine_ls_matrix_type            full
_refine_ls_weighting_scheme
 'calc w=1/[\s^2^(Fo^2^)+(0.0342P)^2^+0.1848P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary    difmap
_atom_sites_solution_hydrogens    geom
_refine_ls_hydrogen_treatment     calc
_refine_ls_extinction_method      none
_refine_ls_extinction_coef        ?
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 'Flack H D (1983), Acta Cryst. A39, 876-881'
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O1 O 0.48781(14) -0.38782(15) 0.53440(10) 0.0344(3) Uani 1 d . . .
O2 O -0.39000(12) -0.31602(14) 0.09468(10) 0.0282(3) Uani 1 d . . .
O3 O -0.23256(11) -0.38268(12) -0.04679(9) 0.0213(2) Uani 1 d . . .
C1 C 0.36975(17) -0.33682(18) 0.44523(13) 0.0228(3) Uani 1 d . . .
C2 C 0.24127(18) -0.21742(19) 0.46287(14) 0.0248(3) Uani 1 d . . .
H2A H 0.2695 -0.1083 0.4399 0.030 Uiso 1 calc R . .
H2B H 0.2332 -0.2184 0.5577 0.030 Uiso 1 calc R . .
C3 C 0.07776(16) -0.27550(16) 0.36172(13) 0.0178(3) Uani 1 d . . .
H3 H 0.0258 -0.3549 0.4103 0.021 Uiso 1 calc R . .
C4 C 0.12930(15) -0.36589(16) 0.24529(12) 0.0159(2) Uani 1 d . . .
C5 C 0.32301(16) -0.38677(17) 0.29567(13) 0.0194(3) Uani 1 d . . .
H5 H 0.3719 -0.3053 0.2467 0.023 Uiso 1 calc R . .
C6 C 0.3966(2) -0.5464(2) 0.27360(15) 0.0280(3) Uani 1 d . . .
H6A H 0.3595 -0.6284 0.3267 0.042 Uiso 1 calc R . .
H6B H 0.5193 -0.5397 0.3035 0.042 Uiso 1 calc R . .
H6C H 0.3586 -0.5740 0.1763 0.042 Uiso 1 calc R . .
C7 C -0.06173(17) -0.15340(17) 0.28846(14) 0.0202(3) Uani 1 d . . .
C8 C -0.10656(16) -0.20614(16) 0.13532(13) 0.0180(3) Uani 1 d . . .
H8 H -0.1520 -0.1138 0.0740 0.022 Uiso 1 calc R . .
C9 C 0.06610(16) -0.25508(16) 0.12182(12) 0.0173(3) Uani 1 d . . .

H9A H 0.0558 -0.3119 0.0348 0.021 Uiso 1 calc R . .
H9B H 0.1405 -0.1617 0.1281 0.021 Uiso 1 calc R . .
C10 C 0.03196(17) -0.52340(16) 0.21189(13) 0.0191(3) Uani 1 d . . .
H10A H 0.0551 -0.5731 0.1313 0.023 Uiso 1 calc R . .
H10B H 0.0711 -0.5975 0.2900 0.023 Uiso 1 calc R . .
C11 C -0.15749(17) -0.49741(17) 0.18222(14) 0.0217(3) Uani 1 d . . .
H11A H -0.2170 -0.5930 0.1356 0.026 Uiso 1 calc R . .
H11B H -0.1845 -0.4855 0.2700 0.026 Uiso 1 calc R . .
C12 C -0.22195(15) -0.35106(17) 0.09334(12) 0.0187(3) Uani 1 d . . .
C13 C 0.0032(2) 0.01919(18) 0.29620(16) 0.0285(3) Uani 1 d . . .
H13A H 0.0436 0.0524 0.3921 0.043 Uiso 1 calc R . .
H13B H -0.0880 0.0898 0.2470 0.043 Uiso 1 calc R . .
H13C H 0.0952 0.0252 0.2544 0.043 Uiso 1 calc R . .
C14 C -0.20761(19) -0.1541(2) 0.35246(15) 0.0290(3) Uani 1 d . . .
H14A H -0.2968 -0.0836 0.3000 0.043 Uiso 1 calc R . .
H14B H -0.1677 -0.1165 0.4471 0.043 Uiso 1 calc R . .
H14C H -0.2513 -0.2627 0.3511 0.043 Uiso 1 calc R . .
C15 C -0.50198(17) -0.3494(2) -0.03632(14) 0.0278(3) Uani 1 d . . .
H15A H -0.5449 -0.2496 -0.0857 0.033 Uiso 1 calc R . .
H15B H -0.5981 -0.4140 -0.0281 0.033 Uiso 1 calc R . .
C16 C -0.39759(17) -0.44162(18) -0.10957(14) 0.0240(3) Uani 1 d . . .
H16A H -0.4044 -0.5577 -0.0949 0.029 Uiso 1 calc R . .
H16B H -0.4335 -0.4192 -0.2089 0.029 Uiso 1 calc R . .

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O2 0.0149(4) 0.0447(7) 0.0232(5) -0.0074(5) 0.0027(4) 0.0014(4)
O3 0.0174(4) 0.0292(5) 0.0151(4) -0.0035(4) 0.0009(3) 0.0002(4)
C1 0.0197(6) 0.0237(7) 0.0214(6) -0.0011(6) 0.0003(5) -0.0057(6)
C2 0.0225(7) 0.0278(7) 0.0198(7) -0.0071(6) -0.0005(5) -0.0015(6)
C3 0.0178(6) 0.0204(6) 0.0147(6) -0.0011(5) 0.0040(5) -0.0010(5)
C4 0.0157(5) 0.0168(6) 0.0141(5) -0.0002(5) 0.0025(4) 0.0003(5)
C5 0.0157(6) 0.0227(6) 0.0182(6) 0.0010(5) 0.0023(5) -0.0009(5)

C6 0.0214(7) 0.0337(8) 0.0251(7) -0.0029(6) 0.0008(6) 0.0085(6)
C7 0.0195(6) 0.0233(7) 0.0169(6) -0.0030(5) 0.0038(5) 0.0014(5)
C8 0.0194(6) 0.0186(6) 0.0152(6) 0.0004(5) 0.0037(5) 0.0030(5)
C9 0.0178(6) 0.0180(6) 0.0152(6) 0.0014(5) 0.0035(5) -0.0010(5)
C10 0.0208(7) 0.0164(6) 0.0178(6) -0.0001(5) 0.0020(5) -0.0024(5)
C11 0.0192(7) 0.0232(7) 0.0209(6) 0.0013(5) 0.0028(5) -0.0057(5)
C12 0.0146(6) 0.0255(7) 0.0154(6) -0.0021(5) 0.0032(4) 0.0000(5)
C13 0.0332(8) 0.0205(7) 0.0293(7) -0.0049(6) 0.0050(6) 0.0028(6)
C14 0.0244(7) 0.0427(9) 0.0206(7) -0.0064(6) 0.0077(6) 0.0055(7)
C15 0.0169(6) 0.0384(9) 0.0239(7) -0.0012(6) -0.0011(5) 0.0002(6)
C16 0.0198(7) 0.0267(7) 0.0208(6) -0.0027(5) -0.0015(5) -0.0024(6)

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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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C1 C5 1.5226(18) . ?
C2 C3 1.5332(18) . ?
C2 H2A 0.9900 . ?
C2 H2B 0.9900 . ?
C3 C7 1.5684(19) . ?
C3 C4 1.5706(17) . ?

C3 H3 1.0000 . ?
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C4 C5 1.5560(17) . ?
C5 C6 1.516(2) . ?
C5 H5 1.0000 . ?
C6 H6A 0.9800 . ?
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C6 H6C 0.9800 . ?
C7 C14 1.5360(19) . ?
C7 C13 1.540(2) . ?
C7 C8 1.5638(18) . ?
C8 C12 1.5330(18) . ?
C8 C9 1.5393(17) . ?
C8 H8 1.0000 . ?
C9 H9A 0.9900 . ?
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C10 H10B 0.9900 . ?
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C13 H13A 0.9800 . ?
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C14 H14B 0.9800 . ?
C14 H14C 0.9800 . ?
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C1 C2 H2B 111.1 . . ?
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H2A C2 H2B 109.1 . . ?
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C4 C3 H3 107.8 . . ?
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C5 C6 H6B 109.5 . . ?
H6A C6 H6B 109.5 . . ?
C5 C6 H6C 109.5 . . ?
H6A C6 H6C 109.5 . . ?
H6B C6 H6C 109.5 . . ?
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C14 C7 C8 115.70(11) . . ?

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O3 C12 C11 110.75(11) . . ?
O2 C12 C11 109.64(11) . . ?
O3 C12 C8 106.26(10) . . ?
O2 C12 C8 111.70(11) . . ?
C11 C12 C8 112.72(10) . . ?
C7 C13 H13A 109.5 . . ?
C7 C13 H13B 109.5 . . ?
H13A C13 H13B 109.5 . . ?
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H13A C13 H13C 109.5 . . ?
H13B C13 H13C 109.5 . . ?

C7 C14 H14A 109.5 . . ?
C7 C14 H14B 109.5 . . ?
H14A C14 H14B 109.5 . . ?
C7 C14 H14C 109.5 . . ?
H14A C14 H14C 109.5 . . ?
H14B C14 H14C 109.5 . . ?
O2 C15 C16 104.56(11) . . ?
O2 C15 H15A 110.8 . . ?
C16 C15 H15A 110.8 . . ?
O2 C15 H15B 110.8 . . ?
C16 C15 H15B 110.8 . . ?
H15A C15 H15B 108.9 . . ?
O3 C16 C15 102.51(11) . . ?
O3 C16 H16A 111.3 . . ?
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O1 C1 C5 C6 20.6(2) . . . . ?
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