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data_a

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_chemical_name_systematic
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_chemical_name_common             ?
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_chemical_formula_moiety          ?
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 'C22 H16 Mn2 N4 O10'
_chemical_formula_weight          606.27

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 _atom_type_scat_dispersion_real
 _atom_type_scat_dispersion_imag
 _atom_type_scat_source
 'C'  'C'   0.0033   0.0016
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 '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'
 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'O'  'O'   0.0106   0.0060
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Mn'  'Mn'   0.3368   0.7283
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

_symmetry_cell_setting            Rhombohedral
_symmetry_space_group_name_H-M    R3c

loop_
 _symmetry_equiv_pos_as_xyz
 'x, y, z'
 '-y, x-y, z'
 '-x+y, -x, z'
 '-y, -x, z+1/2'
 '-x+y, y, z+1/2'
 'x, x-y, z+1/2'
 'x+2/3, y+1/3, z+1/3'
```

'-y+2/3, x-y+1/3, z+1/3'

'-x+y+2/3, -x+1/3, z+1/3'

'-y+2/3, -x+1/3, z+5/6'

'-x+y+2/3, y+1/3, z+5/6'

'x+2/3, x-y+1/3, z+5/6'

'x+1/3, y+2/3, z+2/3'

'-y+1/3, x-y+2/3, z+2/3'

'-x+y+1/3, -x+2/3, z+2/3'

'-y+1/3, -x+2/3, z+7/6'

'-x+y+1/3, y+2/3, z+7/6'

'x+1/3, x-y+2/3, z+7/6'

_cell_length_a	28.5972(6)
_cell_length_b	28.5972(6)
_cell_length_c	8.7442(5)
_cell_angle_alpha	90.00
_cell_angle_beta	90.00
_cell_angle_gamma	120.00
_cell_volume	6192.9(4)
_cell_formula_units_Z	9
_cell_measurement_temperature	296(2)
_cell_measurement_reflns_used	866

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_cell_measurement_theta_min       2.47

_cell_measurement_theta_max       15.60


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_exptl_crystal_colour             yellow

_exptl_crystal_size_max           0.32

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_exptl_crystal_size_min           0.11

_exptl_crystal_density_meas       ?

_exptl_crystal_density_diffrn     1.463

_exptl_crystal_density_method     'not measured'

_exptl_crystal_F_000              2754

_exptl_absorpt_coefficient_mu     0.975

_exptl_absorpt_correction_type    multi-scan

_exptl_absorpt_correction_T_min   0.7456

_exptl_absorpt_correction_T_max   0.9004

_exptl_absorpt_process_details    sadabs


_exptl_special_details

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_diffrn_radiation_type	MoK\a
_diffrn_radiation_source	'fine-focus sealed tube'
_diffrn_radiation_monochromator	graphite
_diffrn_measurement_device_type	'CCD area detector'
_diffrn_measurement_method	'phi and omega scans'
_diffrn_detector_area_resol_mean	?
_diffrn_standards_number	0
_diffrn_standards_interval_count	0
_diffrn_standards_interval_time	0
_diffrn_standards_decay_%	0
_diffrn_reflns_number	9826
_diffrn_reflns_av_R_equivalents	0.1130
_diffrn_reflns_av_sigmaI/netI	0.1825
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_diffrn_reflns_limit_h_max	34
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_diffrn_reflns_limit_k_max	29
_diffrn_reflns_limit_l_min	-10
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_reflns_number_gt                 1242
_reflns_threshold_expression      >2sigma(I)

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_computing_cell_refinement        'Bruker SMART'
_computing_data_reduction         'Bruker SAINT'
_computing_structure_solution     'SHELXS-97 (Sheldrick, 1990)'
_computing_structure_refinement   'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics     'Bruker SHELXTL'
_computing_publication_material   'Bruker SHELXTL'

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

factors based on ALL data will be even larger.

;

_refine_ls_structure_factor_coef Fsqd

_refine_ls_matrix_type full

_refine_ls_weighting_scheme calc

_refine_ls_weighting_details

'calc w=1/[\s^2^(Fo^2^)+(0.0000P)^2^+0.0000P] where P=(Fo^2^+2Fc^2^)/3'

_atom_sites_solution_primary direct

_atom_sites_solution_secondary difmap

_atom_sites_solution_hydrogens geom

_refine_ls_hydrogen_treatment constr

_refine_ls_extinction_method none

_refine_ls_extinction_coef ?

_refine_ls_abs_structure_details

'Flack H D (1983), Acta Cryst. A39, 876-881'

_refine_ls_abs_structure_Flack 0.04(3)

_refine_ls_number_reflns 2544

_refine_ls_number_parameters 172

_refine_ls_number_restraints 1

_refine_ls_R_factor_all 0.1059

_refine_ls_R_factor_gt 0.0515

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_refine_ls_wR_factor_ref          0.0767

_refine_ls_wR_factor_gt           0.0706

_refine_ls_goodness_of_fit_ref    0.879

_refine_ls_restrained_S_all       0.879

_refine_ls_shift/su_max           0.000

_refine_ls_shift/su_mean          0.000



loop_

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 _atom_site_type_symbol

 _atom_site_fract_x

 _atom_site_fract_y

 _atom_site_fract_z

 _atom_site_U_iso_or_equiv

 _atom_site_adp_type

 _atom_site_occupancy

 _atom_site_symmetry_multiplicity

 _atom_site_calc_flag

 _atom_site_refinement_flags

 _atom_site_disorder_assembly

 _atom_site_disorder_group

Mn1 Mn 0.90688(4) 0.24168(4) 0.95029(14) 0.0344(3) Uani 1 1 d . . .
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O1 O 0.8817(2) 0.18134(19) 0.7706(5) 0.0447(15) Uani 1 1 d . . .

O2 O 0.81950(18) 0.12178(19) 0.6263(5) 0.0401(13) Uani 1 1 d . . .

O3 O 0.70146(17) 0.07043(18) 0.6304(6) 0.0506(15) Uani 1 1 d . . .

O4 O 0.65017(17) 0.07126(19) 0.8193(5) 0.0418(14) Uani 1 1 d . . .

O5 O 0.94454(19) 0.30722(18) 0.7828(5) 0.0612(17) Uani 1 1 d . . .

H1W H 0.9809 0.3167 0.7808 0.092 Uiso 1 1 d R . .

H2W H 0.9331 0.3281 0.7953 0.092 Uiso 1 1 d R . .

N1 N 0.8175(2) 0.2146(2) 0.8948(6) 0.0363(15) Uani 1 1 d . . .

N2 N 0.7288(2) 0.1697(2) 0.9154(6) 0.0360(16) Uani 1 1 d . . .

H2 H 0.6969 0.1613 0.9458 0.043 Uiso 1 1 calc R . .

C1 C 0.7960(3) 0.1684(3) 0.8074(7) 0.0306(18) Uani 1 1 d . . .

C2 C 0.7403(3) 0.1388(3) 0.8171(8) 0.0315(19) Uani 1 1 d . . .

C3 C 0.7745(3) 0.2147(3) 0.9564(8) 0.039(2) Uani 1 1 d . . .

C4 C 0.8349(4) 0.1575(3) 0.7330(8) 0.034(2) Uani 1 1 d . . .

C5 C 0.6937(3) 0.0907(3) 0.7581(9) 0.032(2) Uani 1 1 d . . .

C6 C 0.7775(3) 0.2606(3) 1.0499(9) 0.046(2) Uani 1 1 d . . .

C7 C 0.7315(3) 0.2492(3) 1.1427(8) 0.051(2) Uani 1 1 d . . .

H7 H 0.7019 0.2147 1.1535 0.061 Uiso 1 1 calc R . .

C8 C 0.7350(4) 0.2935(4) 1.2139(10) 0.065(3) Uani 1 1 d . . .

H8 H 0.7055 0.2894 1.2701 0.078 Uiso 1 1 calc R . .

C9 C 0.7788(4) 0.3422(4) 1.2061(11) 0.081(3) Uani 1 1 d . . .

H9 H 0.7808 0.3700 1.2666 0.097 Uiso 1 1 calc R . .

C10 C 0.8213(4) 0.3526(4) 1.1098(12) 0.073(3) Uani 1 1 d . . .

H10 H 0.8498 0.3877 1.0965 0.088 Uiso 1 1 calc R . .

C11 C 0.8209(4) 0.3120(3) 1.0373(9) 0.052(2) Uani 1 1 d . . .

H11 H 0.8503 0.3182 0.9771 0.062 Uiso 1 1 calc R . .

loop_

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 _atom_site_aniso_U_11

 _atom_site_aniso_U_22

 _atom_site_aniso_U_33

 _atom_site_aniso_U_23

 _atom_site_aniso_U_13

 _atom_site_aniso_U_12

Mn1 0.0289(8) 0.0385(8) 0.0306(5) -0.0028(7) 0.0002(7) 0.0129(6)

O1 0.024(3) 0.070(4) 0.041(3) -0.020(3) -0.010(3) 0.024(3)

O2 0.035(3) 0.036(4) 0.050(3) -0.004(3) 0.002(3) 0.018(3)

O3 0.029(3) 0.047(4) 0.055(4) -0.007(3) 0.008(3) 0.003(3)

O4 0.025(3) 0.050(4) 0.033(3) -0.007(3) 0.013(3) 0.006(3)

O5 0.065(4) 0.073(4) 0.060(4) 0.025(3) 0.022(3) 0.045(4)

N1 0.036(4) 0.034(4) 0.037(4) -0.001(3) 0.008(3) 0.016(3)

N2 0.022(4) 0.049(4) 0.032(4) -0.001(3) -0.002(3) 0.015(4)

C1 0.035(5) 0.030(5) 0.027(4) -0.006(4) 0.002(4) 0.017(4)

C2 0.027(5) 0.044(5) 0.035(4) -0.007(4) 0.007(4) 0.026(5)

C3 0.029(5) 0.054(6) 0.035(4) 0.018(5) 0.000(4) 0.022(5)

C4 0.029(5) 0.042(6) 0.031(5) -0.009(4) -0.007(4) 0.017(5)

C5 0.018(5) 0.025(5) 0.050(5) -0.005(4) 0.003(4) 0.008(4)

C6 0.065(7) 0.048(6) 0.045(5) -0.026(5) -0.016(5) 0.043(6)

C7 0.052(6) 0.059(7) 0.054(6) -0.019(5) 0.001(5) 0.037(5)

C8 0.052(7) 0.069(7) 0.088(7) -0.036(6) -0.020(6) 0.041(6)

C9 0.096(10) 0.071(8) 0.105(9) -0.035(7) -0.020(7) 0.063(8)

C10 0.090(9) 0.036(7) 0.098(9) 0.000(7) 0.017(7) 0.035(6)

C11 0.055(7) 0.031(5) 0.067(7) 0.006(5) 0.006(5) 0.020(5)

_geom_special_details

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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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loop_

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_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Mn1 O3 2.119(5) 4_665 ?

Mn1 O4 2.160(4) 18_544 ?

Mn1 O2 2.161(5) 4_665 ?

Mn1 O1 2.173(4) . ?

Mn1 O5 2.191(4) . ?

Mn1 N1 2.321(6) . ?

O1 C4 1.205(8) . ?

O2 C4 1.287(8) . ?

O2 Mn1 2.161(5) 4_664 ?

O3 C5 1.327(8) . ?

O3 Mn1 2.119(5) 4_664 ?

O4 C5 1.205(7) . ?

O4 Mn1 2.160(4) 12_444 ?

O5 H1W 0.9349 . ?

O5 H2W 0.8200 . ?

N1 C3 1.344(7) . ?

N1 C1 1.375(7) . ?

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N2 C3 1.347(7) . ?

N2 C2 1.384(7) . ?

N2 H2 0.8600 . ?

C1 C2 1.383(9) . ?

C1 C4 1.450(10) . ?

C2 C5 1.450(8) . ?

C3 C6 1.512(9) . ?

C6 C11 1.376(10) . ?

C6 C7 1.437(9) . ?

C7 C8 1.371(9) . ?

C7 H7 0.9300 . ?

C8 C9 1.330(11) . ?

C8 H8 0.9300 . ?

C9 C10 1.385(11) . ?

C9 H9 0.9300 . ?

C10 C11 1.318(10) . ?

C10 H10 0.9300 . ?

C11 H11 0.9300 . ?


loop_

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O3 Mn1 O4 86.53(19) 4_665 18_544 ?

O3 Mn1 O2 86.47(19) 4_665 4_665 ?

O4 Mn1 O2 84.45(18) 18_544 4_665 ?

O3 Mn1 O1 178.1(2) 4_665 . ?

O4 Mn1 O1 94.06(18) 18_544 . ?

O2 Mn1 O1 91.79(18) 4_665 . ?

O3 Mn1 O5 90.54(18) 4_665 . ?

O4 Mn1 O5 90.02(17) 18_544 . ?

O2 Mn1 O5 173.86(19) 4_665 . ?

O1 Mn1 O5 91.26(19) . . ?

O3 Mn1 N1 106.0(2) 4_665 . ?

O4 Mn1 N1 165.13(19) 18_544 . ?

O2 Mn1 N1 88.27(17) 4_665 . ?

O1 Mn1 N1 73.18(19) . . ?

O5 Mn1 N1 97.71(18) . . ?

C4 O1 Mn1 118.7(5) . . ?

C4 O2 Mn1 135.0(5) . 4_664 ?

C5 O3 Mn1 139.6(4) . 4_664 ?

C5 O4 Mn1 134.2(5) . 12_444 ?

Mn1 O5 H1W 105.1 . . ?

Mn1 O5 H2W 109.3 . . ?

H1W O5 H2W 125.7 . . ?

C3 N1 C1 104.8(6) . . ?

C3 N1 Mn1 140.4(5) . . ?

C1 N1 Mn1 109.0(5) . . ?

C3 N2 C2 110.3(6) . . ?

C3 N2 H2 124.8 . . ?

C2 N2 H2 124.8 . . ?

N1 C1 C2 112.2(7) . . ?

N1 C1 C4 115.7(7) . . ?

C2 C1 C4 131.9(7) . . ?

C1 C2 N2 102.5(6) . . ?

C1 C2 C5 142.2(7) . . ?

N2 C2 C5 115.2(6) . . ?

N1 C3 N2 110.0(7) . . ?

N1 C3 C6 124.4(7) . . ?

N2 C3 C6 125.4(7) . . ?

O1 C4 O2 119.3(8) . . ?

O1 C4 C1 120.6(8) . . ?

O2 C4 C1 120.1(7) . . ?

O4 C5 O3 122.1(7) . . ?

O4 C5 C2 121.9(7) . . ?

O3 C5 C2 116.0(6) . . ?

C11 C6 C7 121.5(7) . . ?

C11 C6 C3 120.9(8) . . ?

C7 C6 C3 117.5(8) . . ?

C8 C7 C6 114.3(8) . . ?

C8 C7 H7 122.8 . . ?

C6 C7 H7 122.8 . . ?

C9 C8 C7 122.7(9) . . ?

C9 C8 H8 118.6 . . ?

C7 C8 H8 118.6 . . ?

C8 C9 C10 121.5(9) . . ?

C8 C9 H9 119.3 . . ?

C10 C9 H9 119.3 . . ?

C11 C10 C9 119.0(8) . . ?

C11 C10 H10 120.5 . . ?

C9 C10 H10 120.5 . . ?

C10 C11 C6 120.6(8) . . ?

C10 C11 H11 119.7 . . ?

C6 C11 H11 119.7 . . ?

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loop_
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 _geom_torsion_site_symmetry_2
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 _geom_torsion_publ_flag
O3 Mn1 O1 C4 57(6) 4_665 . . . ?
O4 Mn1 O1 C4 165.1(5) 18_544 . . . ?
O2 Mn1 O1 C4 80.6(5) 4_665 . . . ?
O5 Mn1 O1 C4 -104.8(5) . . . . ?
N1 Mn1 O1 C4 -7.1(5) . . . . ?
O3 Mn1 N1 C3 -17.7(8) 4_665 . . . ?
O4 Mn1 N1 C3 128.7(8) 18_544 . . . ?
O2 Mn1 N1 C3 68.1(7) 4_665 . . . ?
O1 Mn1 N1 C3 160.5(8) . . . . ?
O5 Mn1 N1 C3 -110.5(7) . . . . ?
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O3 Mn1 N1 C1 -165.0(4) 4_665 . . . ?

O4 Mn1 N1 C1 -18.5(10) 18_544 . . . ?

O2 Mn1 N1 C1 -79.1(4) 4_665 . . . ?

O1 Mn1 N1 C1 13.2(4) . . . . ?

O5 Mn1 N1 C1 102.2(4) . . . . ?

C3 N1 C1 C2 -1.8(7) . . . . ?

Mn1 N1 C1 C2 157.3(4) . . . . ?

C3 N1 C1 C4 -177.3(5) . . . . ?

Mn1 N1 C1 C4 -18.2(6) . . . . ?

N1 C1 C2 N2 0.2(7) . . . . ?

C4 C1 C2 N2 174.7(6) . . . . ?

N1 C1 C2 C5 177.4(9) . . . . ?

C4 C1 C2 C5 -8.1(15) . . . . ?

C3 N2 C2 C1 1.5(7) . . . . ?

C3 N2 C2 C5 -176.6(6) . . . . ?

C1 N1 C3 N2 2.8(7) . . . . ?

Mn1 N1 C3 N2 -145.3(6) . . . . ?

C1 N1 C3 C6 -173.8(6) . . . . ?

Mn1 N1 C3 C6 38.2(11) . . . . ?

C2 N2 C3 N1 -2.8(8) . . . . ?

C2 N2 C3 C6 173.7(6) . . . . ?

Mn1 O1 C4 O2 179.8(4) . . . . ?

Mn1 O1 C4 C1 -0.7(9) . . . . ?

Mn1 O2 C4 O1 -148.0(5) 4_664 . . . ?

Mn1 O2 C4 C1 32.4(10) 4_664 . . . ?

N1 C1 C4 O1 14.0(9) . . . . ?

C2 C1 C4 O1 -160.3(7) . . . . ?

N1 C1 C4 O2 -166.4(6) . . . . ?

C2 C1 C4 O2 19.3(11) . . . . ?

Mn1 O4 C5 O3 8.0(12) 12_444 . . . ?

Mn1 O4 C5 C2 -174.1(5) 12_444 . . . ?

Mn1 O3 C5 O4 162.6(5) 4_664 . . . ?

Mn1 O3 C5 C2 -15.4(11) 4_664 . . . ?

C1 C2 C5 O4 164.0(9) . . . . ?

N2 C2 C5 O4 -19.0(10) . . . . ?

C1 C2 C5 O3 -17.9(14) . . . . ?

N2 C2 C5 O3 159.0(6) . . . . ?

N1 C3 C6 C11 21.7(11) . . . . ?

N2 C3 C6 C11 -154.3(7) . . . . ?

N1 C3 C6 C7 -162.9(7) . . . . ?

N2 C3 C6 C7 21.1(10) . . . . ?

C11 C6 C7 C8 0.7(11) . . . . ?

C3 C6 C7 C8 -174.7(6) . . . . ?

C6 C7 C8 C9 -4.4(12) . . . . ?

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C7 C8 C9 C10 8.0(15) . . . . ?

C8 C9 C10 C11 -7.5(15) . . . . ?

C9 C10 C11 C6 3.8(14) . . . . ?

C7 C6 C11 C10 -0.6(12) . . . . ?

C3 C6 C11 C10 174.6(8) . . . . ?


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 _geom_hbond_atom_site_label_H

 _geom_hbond_atom_site_label_A

 _geom_hbond_distance_DH

 _geom_hbond_distance_HA

 _geom_hbond_distance_DA

 _geom_hbond_angle_DHA

 _geom_hbond_site_symmetry_A

O5 H1W O3  0.93 1.88 2.730(6) 150.5 18_544


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_diffrn_reflns_theta_full              25.50

_diffrn_measured_fraction_theta_full   0.999

_refine_diff_density_max    0.493

_refine_diff_density_min   -0.353
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_refine_diff_density_rms 0.071