University of Groningen

The role of salicylic acid, L-ascorbic acid and oxalic acid in promoting the oxidation of alkenes with H₂O₂ catalysed by [Mn(IV) (2)(O)₃(tmtacn)₂](2+)

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_publ_contact_author_email B.L.FERINGA@RUG.NL

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;
The role of salicylic acid, L-ascorbic acid and oxalic
acid in promoting the oxidation of alkenes with H2O2 catalysed by
[MnIV2(O)3(tmtacn)2]2+
;
loop_
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'Paul Alsters'
'Wesley Browne'
'Johannes W. de Boer'
'Ronald Hage'
'Auke Meetsma'

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0. AUDIT DETAILS

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4. TEXT

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;
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Insert blank lines between paragraphs

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The asymmetric unit consists of five moieties:

a cationic dinuclear Mn-complex, two anionic hexafluoridephosphides and two disordered, half ethylacetate solvent molecules.

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;
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_publ_section_exptl_refinement
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;
The structure was solved by Patterson methods and extension of the model was accomplished by direct methods applied to difference structure factors using the program DIRDIF.8 The positional and anisotropic displacement parameters for the non-hydrogen atoms were refined. Refinement was frustrated by a disorder problem: from the solution it was clear that the two ethylacetate solvent molecules were highly disordered, each over an inversion center. No satisfactory discrete model could be fitted in this density. The BYPASS procedure was used to squeeze out the disordered cyclohexane solvent molecule. Hydrogen atoms were constrained to idealized geometries and allowed to ride on their carrier atoms with an isotropic displacement parameter related to the equivalent displacement parameter of their carrier atoms.
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Beurskens, P.T., Beurskens, G., Gelder, R. de Garc'ia-Granda, S. Gould, R.O. Isra'el, & Smits, J.M.M. (1999). The DIRDIF99 program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

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;

Fig. 1. Chemical structural diagram (scheme 1) of the title compound

Fig. 2. Perspective PLUTO drawing of the molecule illustrating the configuration and the adopted numbering scheme.

Fig. 3. Molecular packing viewed down unit cell axes.

Fig. 4. Perspective ORTEP drawing of the title compound. Displacement ellipsoids for non-H are represented at the 50% probability level.

The H-atoms have been omitted to improve clarity.

;

#=====

5. CHEMICAL DATA

_chemical_name_systematic

; ?

;

_chemical_name_common

?

_chemical_melting_point

?

_chemical_formula_moiety

'C32 H52 Mn2 N6 O5, 2(F6 P), 2(C4 H8 O2)0.5'

Ex: 'C12 H16 N2 O6, H2 O' and '(Cd 2+)₃, (C6 N6 Cr 3-)₂, 2(H2 O)'

_chemical_formula_structural

?

_chemical_formula_sum

'C36 H60 F12 Mn2 N6 O5 P2'

_chemical_formula_iupac

?

_chemical_formula_weight

1088.71

_chemical_compound_source

'see text'

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scatter_dispersion_real

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P P 0.1023 0.0942 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

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N N 0.0061 0.0033 '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'

F F 0.0171 0.0103 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

H H 0.0000 0.0000 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

C C 0.0033 0.0016 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'

#=====

6. CRYSTAL DATA

_symmetry_cell_setting

Triclinic

```

_symmetry_space_group_name_Hall '-P 1'
_symmetry_space_group_name_H-M 'P -1'
_symmetry_Int_Tables_number 2

loop_
_symmetry_equiv_pos_as_xyz
x,y,z
-x,-y,-z

_cell_length_a 11.4974(5)
_cell_length_b 13.7430(6)
_cell_length_c 16.3508(7)
_cell_angle_alpha 76.826(1)
_cell_angle_beta 76.090(1)
_cell_angle_gamma 69.359(1)
_cell_volume 2317.49(17)
_cell_formula_units_Z 2

_cell_measurement_temperature 100(1)
_cell_measurement_reflns_used 7227
_cell_measurement_theta_min 2.22
_cell_measurement_theta_max 29.76
_cell_special_details
;
The final unit cell was obtained from the xyz centroids of
7227 reflections after integration using the SAINT software
package (Bruker, 2000).
;

_exptl_crystal_description block
_exptl_crystal_colour violet
_exptl_crystal_size_max 0.50
_exptl_crystal_size_mid 0.47
_exptl_crystal_size_min 0.41
_exptl_crystal_size_rad ?
_exptl_crystal_density_meas ?
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_exptl_crystal_F_000 1124
_exptl_absorpt_coefficient_mu 0.714
_exptl_absorpt_correction_type Multi-Scan
_exptl_absorpt_process_details '(SADABS, Sheldrick, Bruker, 2001))'
_exptl_absorpt_correction_T_min 0.6874
_exptl_absorpt_correction_T_max 0.7612

#=====

# 7. EXPERIMENTAL DATA

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_diffn_radiation_wavelength 0.71073
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_diffn_radiation_source 'fine focus sealed Siemens Mo tube '
_diffn_radiation_monochromator 'parallel mounted graphite'
_diffn_radiation_detector
;
CCD area-detector
;

```

```

_diffrn_measurement_device_type
;
Bruker Smart Apex
;
_diffrn_measurement_method      'phi and omega scans'
_diffrn_special_details
;
Crystal into the cold nitrogen stream of the low-temperature unit
(KRYOFLEX, (Bruker, 2000)).
;
_diffrn_detector_area_resol_mean 66.06

_diffrn_standards_number        ?
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_diffrn_standards_interval_time ?

loop_
_diffrn_standard_refl_index_h
_diffrn_standard_refl_index_k
_diffrn_standard_refl_index_l
? ? ?

# number of measured reflections (redundant set)
_diffrn_reflns_number           22101
_diffrn_reflns_av_R_equivalents 0.0139
_diffrn_reflns_av_sigmaI/netI   0.0229
_diffrn_reflns_limit_h_min      -14
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_diffrn_reflns_limit_k_min      -17
_diffrn_reflns_limit_k_max      18
_diffrn_reflns_limit_l_min      -21
_diffrn_reflns_limit_l_max      21
_diffrn_reflns_theta_min        2.22
_diffrn_reflns_theta_max        28.28
_diffrn_measured_fraction_theta_max 0.960
_diffrn_reflns_theta_full       25.00
_diffrn_measured_fraction_theta_full 0.993

_diffrn_reflns_reduction_process
;
Intensity data were corrected for Lorentz and polarization
effects, decay and absorption and reduced to  $F_o^2$ 
using SAINT (Bruker, 2000) and SADABS (Sheldrick, 2001)
;

# number of unique reflections
_reflns_number_total            11061
_reflns_number_gt               10023
_reflns_threshold_expression      $I > 2\sigma(I)$ 

_computing_data_collection      'SMART, Version 5.624, (Bruker, 2001)'
_computing_cell_refinement      'SAINTPLUS, Version 6.02A, (Bruker, 2000)'
_computing_data_reduction       'XPREP, Version 5.1/NT, (Bruker, 2000)'
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;
DIRDIF-99 (Beurskens et al., 1999)
;
_computing_structure_refinement 'SHELXL-97 (Sheldrick, 1997)'
_computing_molecular_graphics
;
PLUTO (Meetsma, 2003)

```

```

PLATON (Spek, 1994)
;
_computing_publication_material 'PLATON (Spek, 2003)'

#=====

# 8. REFINEMENT DATA

_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^)+(0.0565P)^2^+2.3873P] where P=(Fo^2^+2Fc^2^)/3'
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_atom_sites_solution_secondary direct
_atom_sites_solution_hydrogens geom
_refine_ls_hydrogen_treatment constr
_refine_ls_extinction_method none
_refine_ls_extinction_coef ?
_refine_ls_abs_structure_details ?
_chemical_absolute_configuration ?

_refine_ls_abs_structure_Flack ?
_refine_ls_number_reflns 11061
_refine_ls_number_parameters 538
_refine_ls_number_restraints 0
_refine_ls_number_constraints ?
_refine_ls_R_factor_all 0.0414
_refine_ls_R_factor_gt 0.0384
_refine_ls_wR_factor_ref 0.1078
_refine_ls_wR_factor_gt 0.1052
_refine_ls_goodness_of_fit_ref 1.025
_refine_ls_restrained_S_all 1.025
_refine_ls_shift/su_max 0.001
_refine_ls_shift/su_mean 0.000

_refine_diff_density_max 1.288
_refine_diff_density_min -0.707
_refine_diff_density_rms 0.076

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_vrn_publ_code_frame_time_sec 10.0
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# 9. ATOMIC COORDINATES AND DISPLACEMENT PARAMETERS

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 _atom_site_fract_y
 _atom_site_fract_z
 _atom_site_occupancy
 _atom_site_U_iso_or_equiv
 _atom_site_calc_flag
 _atom_site_refinement_flags

Mn11	Mn	Uani	0.22304(2)	0.14740(2)	0.75793(2)	1.000	0.0137(1)	. .
Mn12	Mn	Uani	0.37715(2)	-0.09619(2)	0.78608(2)	1.000	0.0131(1)	. .
O11	O	Uani	0.24283(11)	0.01184(10)	0.75291(8)	1.000	0.0159(3)	. .
O12	O	Uani	0.23618(12)	0.12204(10)	0.88263(8)	1.000	0.0182(3)	. .
O13	O	Uani	0.37051(12)	-0.04199(10)	0.89679(8)	1.000	0.0185(3)	. .
O14	O	Uani	0.40964(12)	0.13879(10)	0.70930(8)	1.000	0.0194(3)	. .
O15	O	Uani	0.50817(12)	-0.03393(10)	0.70999(8)	1.000	0.0189(3)	. .
N11	N	Uani	0.01211(14)	0.19921(12)	0.79628(10)	1.000	0.0188(4)	. .
N12	N	Uani	0.18938(14)	0.30998(12)	0.75635(10)	1.000	0.0174(4)	. .
N13	N	Uani	0.16573(15)	0.21170(13)	0.63161(10)	1.000	0.0209(4)	. .
N14	N	Uani	0.26747(14)	-0.20209(12)	0.85422(10)	1.000	0.0181(4)	. .
N15	N	Uani	0.52475(14)	-0.22971(12)	0.82695(9)	1.000	0.0160(4)	. .
N16	N	Uani	0.40755(15)	-0.19426(12)	0.68480(10)	1.000	0.0194(4)	. .
C11	C	Uani	0.29614(16)	0.03885(14)	0.92637(11)	1.000	0.0153(4)	. .
C12	C	Uani	0.27189(16)	0.03682(14)	1.02077(11)	1.000	0.0163(5)	. .
C13	C	Uani	0.33819(19)	-0.04970(15)	1.07345(12)	1.000	0.0214(5)	. .
C14	C	Uani	0.3078(2)	-0.05397(16)	1.16151(12)	1.000	0.0251(6)	. .
C15	C	Uani	0.21195(19)	0.02724(17)	1.19693(12)	1.000	0.0245(6)	. .
C16	C	Uani	0.14740(18)	0.11458(17)	1.14509(12)	1.000	0.0234(5)	. .
C17	C	Uani	0.17745(17)	0.11991(15)	1.05697(12)	1.000	0.0193(5)	. .
C18	C	Uani	0.50325(16)	0.06176(14)	0.68805(10)	1.000	0.0152(4)	. .
C19	C	Uani	0.61736(16)	0.08417(14)	0.63176(11)	1.000	0.0159(4)	. .
C110	C	Uani	0.62628(17)	0.18522(15)	0.61458(12)	1.000	0.0205(5)	. .
C111	C	Uani	0.73312(19)	0.20489(16)	0.56211(14)	1.000	0.0259(5)	. .
C112	C	Uani	0.82963(18)	0.12390(17)	0.52680(13)	1.000	0.0255(5)	. .
C113	C	Uani	0.82167(17)	0.02287(16)	0.54442(12)	1.000	0.0228(5)	. .
C114	C	Uani	0.71566(17)	0.00250(14)	0.59730(11)	1.000	0.0182(5)	. .
C115	C	Uani	-0.03248(18)	0.11497(16)	0.85390(13)	1.000	0.0245(5)	. .
C116	C	Uani	-0.01262(17)	0.28704(14)	0.84318(12)	1.000	0.0197(5)	. .
C117	C	Uani	0.05372(17)	0.36512(14)	0.79140(12)	1.000	0.0200(5)	. .
C118	C	Uani	0.27356(18)	0.32700(15)	0.80464(13)	1.000	0.0223(5)	. .
C119	C	Uani	0.22150(18)	0.35389(15)	0.66422(12)	1.000	0.0220(5)	. .
C120	C	Uani	0.1498(2)	0.32694(15)	0.61089(12)	1.000	0.0243(5)	. .
C121	C	Uani	0.2588(2)	0.15766(17)	0.56332(13)	1.000	0.0280(6)	. .
C122	C	Uani	0.04466(19)	0.18966(16)	0.64253(13)	1.000	0.0248(5)	. .
C123	C	Uani	-0.04828(18)	0.23358(16)	0.71895(13)	1.000	0.0235(5)	. .
C124	C	Uani	0.16082(18)	-0.15069(16)	0.91755(13)	1.000	0.0248(5)	. .
C125	C	Uani	0.35023(17)	-0.29995(14)	0.89902(12)	1.000	0.0191(5)	. .
C126	C	Uani	0.46681(17)	-0.28037(14)	0.90972(11)	1.000	0.0178(5)	. .
C127	C	Uani	0.62827(17)	-0.19773(15)	0.84146(13)	1.000	0.0208(5)	. .
C128	C	Uani	0.57806(17)	-0.30604(14)	0.76417(12)	1.000	0.0191(5)	. .
C129	C	Uani	0.54419(18)	-0.25391(15)	0.67717(12)	1.000	0.0216(5)	. .
C130	C	Uani	0.3823(2)	-0.13019(17)	0.60196(12)	1.000	0.0283(6)	. .
C131	C	Uani	0.32623(19)	-0.26402(15)	0.71437(13)	1.000	0.0226(5)	. .
C132	C	Uani	0.21903(18)	-0.22329(15)	0.78595(13)	1.000	0.0222(5)	. .
H13	H	Uiso	0.40392	-0.10552	1.04922	1.000	0.0256	. .
H14	H	Uiso	0.35287	-0.11278	1.19748	1.000	0.0301	. .
H15	H	Uiso	0.19027	0.02308	1.25719	1.000	0.0293	. .
H16	H	Uiso	0.08278	0.17067	1.16973	1.000	0.0281	. .
H17	H	Uiso	0.13386	0.17999	1.02129	1.000	0.0232	. .
H110	H	Uiso	0.55971	0.24078	0.63854	1.000	0.0246	. .

H111	H	Uiso	0.73978	0.27386	0.55055	1.000	0.0310	.	.
H112	H	Uiso	0.90175	0.13780	0.49026	1.000	0.0307	.	.
H113	H	Uiso	0.88850	-0.03251	0.52043	1.000	0.0274	.	.
H114	H	Uiso	0.71028	-0.06693	0.60990	1.000	0.0218	.	.
H115	H	Uiso	0.01373	0.08797	0.90174	1.000	0.0368	.	.
H115'	H	Uiso	-0.01780	0.05770	0.82250	1.000	0.0368	.	.
H115"	H	Uiso	-0.12296	0.14332	0.87571	1.000	0.0368	.	.
H116	H	Uiso	0.01756	0.25861	0.89831	1.000	0.0236	.	.
H116'	H	Uiso	-0.10465	0.32340	0.85535	1.000	0.0236	.	.
H117	H	Uiso	0.00913	0.40640	0.74364	1.000	0.0239	.	.
H117'	H	Uiso	0.05053	0.41469	0.82796	1.000	0.0239	.	.
H118	H	Uiso	0.36157	0.28820	0.78390	1.000	0.0334	.	.
H118'	H	Uiso	0.25107	0.30170	0.86552	1.000	0.0334	.	.
H118"	H	Uiso	0.26332	0.40229	0.79623	1.000	0.0334	.	.
H119	H	Uiso	0.31336	0.32446	0.64403	1.000	0.0264	.	.
H119'	H	Uiso	0.19978	0.43133	0.65770	1.000	0.0264	.	.
H120	H	Uiso	0.05913	0.36787	0.62278	1.000	0.0291	.	.
H120'	H	Uiso	0.18205	0.34560	0.54955	1.000	0.0291	.	.
H121	H	Uiso	0.27353	0.08160	0.57856	1.000	0.0420	.	.
H121'	H	Uiso	0.33839	0.17229	0.55657	1.000	0.0420	.	.
H121"	H	Uiso	0.22625	0.18328	0.50959	1.000	0.0420	.	.
H122	H	Uiso	0.06129	0.11265	0.65053	1.000	0.0298	.	.
H122'	H	Uiso	0.00713	0.22167	0.59034	1.000	0.0298	.	.
H123	H	Uiso	-0.07793	0.31145	0.70629	1.000	0.0282	.	.
H123'	H	Uiso	-0.12252	0.20880	0.72994	1.000	0.0282	.	.
H124	H	Uiso	0.11074	-0.08297	0.88968	1.000	0.0372	.	.
H124'	H	Uiso	0.19353	-0.13900	0.96333	1.000	0.0372	.	.
H124"	H	Uiso	0.10752	-0.19605	0.94160	1.000	0.0372	.	.
H125	H	Uiso	0.37517	-0.35791	0.86547	1.000	0.0229	.	.
H125'	H	Uiso	0.30340	-0.32110	0.95567	1.000	0.0229	.	.
H126	H	Uiso	0.44375	-0.23407	0.95331	1.000	0.0214	.	.
H126'	H	Uiso	0.52856	-0.34796	0.92951	1.000	0.0214	.	.
H127	H	Uiso	0.59289	-0.14382	0.87875	1.000	0.0311	.	.
H127'	H	Uiso	0.67085	-0.16917	0.78668	1.000	0.0311	.	.
H127"	H	Uiso	0.68917	-0.25916	0.86850	1.000	0.0311	.	.
H128	H	Uiso	0.54466	-0.36618	0.78544	1.000	0.0229	.	.
H128'	H	Uiso	0.67107	-0.33371	0.75912	1.000	0.0229	.	.
H129	H	Uiso	0.59393	-0.20547	0.64982	1.000	0.0259	.	.
H129'	H	Uiso	0.56573	-0.30828	0.64056	1.000	0.0259	.	.
H130	H	Uiso	0.43190	-0.08144	0.58496	1.000	0.0424	.	.
H130'	H	Uiso	0.29220	-0.09009	0.60673	1.000	0.0424	.	.
H130"	H	Uiso	0.40581	-0.17633	0.55896	1.000	0.0424	.	.
H131	H	Uiso	0.37812	-0.33621	0.73490	1.000	0.0271	.	.
H131'	H	Uiso	0.29068	-0.26720	0.66593	1.000	0.0271	.	.
H132	H	Uiso	0.15772	-0.15771	0.76256	1.000	0.0267	.	.
H132'	H	Uiso	0.17446	-0.27609	0.81036	1.000	0.0267	.	.
P21	P	Uani	0.42113(5)	0.61540(4)	0.16012(3)	1.000	0.0200(1)	.	.
F21	F	Uani	0.52540(12)	0.52434(10)	0.20879(8)	1.000	0.0313(4)	.	.
F22	F	Uani	0.31499(13)	0.56320(10)	0.21234(9)	1.000	0.0369(4)	.	.
F23	F	Uani	0.45134(12)	0.54424(10)	0.08786(8)	1.000	0.0301(4)	.	.
F24	F	Uani	0.31749(11)	0.70576(10)	0.11051(9)	1.000	0.0301(4)	.	.
F25	F	Uani	0.52620(11)	0.66783(10)	0.10698(8)	1.000	0.0290(4)	.	.
F26	F	Uani	0.39099(15)	0.68568(10)	0.23259(8)	1.000	0.0386(4)	.	.
P31	P	Uani	0.01800(5)	0.32356(4)	0.34464(3)	1.000	0.0265(1)	.	.
F31	F	Uani	0.16164(17)	0.26369(15)	0.36068(15)	1.000	0.0679(7)	.	.
F32	F	Uani	-0.0266(2)	0.29473(15)	0.44390(10)	1.000	0.0611(7)	.	.
F33	F	Uani	0.00441(19)	0.21713(12)	0.32953(10)	1.000	0.0526(6)	.	.
F34	F	Uani	-0.11899(16)	0.38403(15)	0.32836(17)	1.000	0.0723(8)	.	.
F35	F	Uani	0.0746(2)	0.35052(17)	0.24640(11)	1.000	0.0716(7)	.	.
F36	F	Uani	0.03106(14)	0.42926(11)	0.36084(10)	1.000	0.0402(5)	.	.

```

loop_
_atom_site_aniso_label
_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
Mn11 0.0137(1) 0.0114(1) 0.0146(1) -0.0025(1) -0.0031(1) -0.0018(1)
Mn12 0.0131(1) 0.0109(1) 0.0142(1) -0.0021(1) -0.0023(1) -0.0025(1)
O11 0.0153(5) 0.0136(6) 0.0181(6) -0.0024(4) -0.0050(4) -0.0025(4)
O12 0.0213(6) 0.0151(6) 0.0161(6) -0.0037(5) -0.0043(5) -0.0018(5)
O13 0.0190(6) 0.0168(6) 0.0180(6) -0.0049(5) -0.0049(5) -0.0012(5)
O14 0.0166(6) 0.0155(6) 0.0240(6) -0.0050(5) 0.0005(5) -0.0042(5)
O15 0.0174(6) 0.0143(6) 0.0209(6) -0.0022(5) 0.0007(5) -0.0032(5)
N11 0.0171(7) 0.0164(7) 0.0223(7) -0.0039(6) -0.0053(6) -0.0030(6)
N12 0.0166(7) 0.0144(7) 0.0197(7) -0.0034(5) -0.0029(5) -0.0028(5)
N13 0.0243(8) 0.0163(7) 0.0200(7) -0.0046(6) -0.0052(6) -0.0019(6)
N14 0.0164(7) 0.0167(7) 0.0205(7) -0.0034(6) -0.0039(5) -0.0035(6)
N15 0.0153(7) 0.0134(7) 0.0187(7) -0.0025(5) -0.0030(5) -0.0039(5)
N16 0.0225(8) 0.0167(7) 0.0181(7) -0.0022(6) -0.0058(6) -0.0039(6)
C11 0.0142(7) 0.0162(8) 0.0167(8) -0.0035(6) -0.0028(6) -0.0058(6)
C12 0.0174(8) 0.0183(8) 0.0154(8) -0.0037(6) -0.0030(6) -0.0074(7)
C13 0.0273(9) 0.0178(9) 0.0208(9) -0.0029(7) -0.0083(7) -0.0067(7)
C14 0.0369(11) 0.0230(9) 0.0205(9) 0.0011(7) -0.0126(8) -0.0134(8)
C15 0.0297(10) 0.0352(11) 0.0158(8) -0.0049(7) -0.0040(7) -0.0184(9)
C16 0.0181(8) 0.0341(11) 0.0219(9) -0.0121(8) -0.0008(7) -0.0099(8)
C17 0.0167(8) 0.0221(9) 0.0195(8) -0.0050(7) -0.0041(6) -0.0049(7)
C18 0.0163(8) 0.0153(8) 0.0135(7) -0.0018(6) -0.0034(6) -0.0041(6)
C19 0.0149(7) 0.0177(8) 0.0144(7) -0.0009(6) -0.0034(6) -0.0048(6)
C110 0.0186(8) 0.0173(8) 0.0242(9) -0.0035(7) -0.0037(7) -0.0040(7)
C111 0.0232(9) 0.0211(9) 0.0339(10) 0.0014(8) -0.0052(8) -0.0111(8)
C112 0.0165(8) 0.0309(10) 0.0267(9) 0.0014(8) -0.0020(7) -0.0094(8)
C113 0.0146(8) 0.0262(10) 0.0231(9) -0.0035(7) -0.0016(7) -0.0022(7)
C114 0.0179(8) 0.0176(8) 0.0173(8) -0.0017(6) -0.0031(6) -0.0040(7)
C115 0.0201(9) 0.0209(9) 0.0316(10) -0.0034(8) -0.0016(7) -0.0078(7)
C116 0.0169(8) 0.0166(8) 0.0232(9) -0.0063(7) -0.0021(6) -0.0014(7)
C117 0.0180(8) 0.0148(8) 0.0237(9) -0.0054(7) -0.0027(7) -0.0003(7)
C118 0.0219(9) 0.0182(9) 0.0293(10) -0.0074(7) -0.0065(7) -0.0058(7)
C119 0.0229(9) 0.0154(8) 0.0226(9) -0.0001(7) -0.0006(7) -0.0040(7)
C120 0.0303(10) 0.0169(9) 0.0202(9) -0.0002(7) -0.0059(7) -0.0016(8)
C121 0.0338(11) 0.0260(10) 0.0195(9) -0.0077(8) -0.0036(8) -0.0019(8)
C122 0.0256(9) 0.0223(9) 0.0274(10) -0.0060(7) -0.0136(8) -0.0015(8)
C123 0.0192(8) 0.0228(9) 0.0290(10) -0.0051(7) -0.0113(7) -0.0019(7)
C124 0.0176(8) 0.0251(10) 0.0277(10) -0.0047(8) 0.0015(7) -0.0053(7)
C125 0.0195(8) 0.0156(8) 0.0209(8) 0.0009(6) -0.0042(6) -0.0058(7)
C126 0.0189(8) 0.0146(8) 0.0180(8) 0.0001(6) -0.0049(6) -0.0036(6)
C127 0.0162(8) 0.0175(8) 0.0290(9) -0.0034(7) -0.0074(7) -0.0037(7)
C128 0.0175(8) 0.0138(8) 0.0236(9) -0.0061(7) -0.0021(7) -0.0012(6)
C129 0.0230(9) 0.0177(8) 0.0216(9) -0.0077(7) -0.0009(7) -0.0027(7)
C130 0.0401(12) 0.0247(10) 0.0191(9) -0.0013(7) -0.0108(8) -0.0068(9)
C131 0.0273(9) 0.0179(9) 0.0266(9) -0.0049(7) -0.0107(7) -0.0071(7)
C132 0.0204(9) 0.0192(9) 0.0297(10) -0.0032(7) -0.0087(7) -0.0071(7)
P21 0.0206(2) 0.0138(2) 0.0245(2) -0.0040(2) -0.0045(2) -0.0031(2)
F21 0.0363(7) 0.0202(6) 0.0365(7) -0.0007(5) -0.0188(5) -0.0021(5)
F22 0.0313(7) 0.0262(7) 0.0473(8) -0.0004(6) 0.0029(6) -0.0117(5)
F23 0.0352(7) 0.0235(6) 0.0343(7) -0.0125(5) -0.0107(5) -0.0045(5)
F24 0.0236(6) 0.0210(6) 0.0416(7) 0.0001(5) -0.0108(5) -0.0018(5)
F25 0.0253(6) 0.0304(7) 0.0342(7) -0.0003(5) -0.0080(5) -0.0133(5)
F26 0.0608(9) 0.0225(6) 0.0294(7) -0.0110(5) -0.0055(6) -0.0068(6)
P31 0.0296(3) 0.0175(2) 0.0232(2) -0.0010(2) -0.0002(2) -0.0006(2)

```

```

F31 0.0386(9) 0.0473(10) 0.0944(15) 0.0057(10) -0.0132(9) 0.0052(8)
F32 0.0976(15) 0.0676(12) 0.0303(8) -0.0085(8) 0.0103(8) -0.0544(11)
F33 0.0877(13) 0.0250(7) 0.0419(8) -0.0117(6) -0.0075(8) -0.0126(8)
F34 0.0381(9) 0.0472(10) 0.141(2) -0.0415(12) -0.0419(11) 0.0090(8)
F35 0.0954(16) 0.0689(13) 0.0337(9) 0.0026(8) 0.0066(9) -0.0241(12)
F36 0.0450(8) 0.0242(7) 0.0532(9) 0.0025(6) -0.0187(7) -0.0118(6)

```

```
#=====
```

``` # 10. MOLECULAR GEOMETRY ```

```
_geom_special_details
```

```
;
```

Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

```
;
```

```
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
```

```
Mn11 O11 1.8142(13) . . yes
```

```
Mn11 O12 2.0220(13) . . yes
```

```
Mn11 O14 2.0719(15) . . yes
```

```
Mn11 N11 2.2442(17) . . yes
```

```
Mn11 N12 2.1240(16) . . yes
```

```
Mn11 N13 2.2120(17) . . yes
```

```
Mn12 O11 1.8173(14) . . yes
```

```
Mn12 O13 2.0846(13) . . yes
```

```
Mn12 O15 2.0178(14) . . yes
```

```
Mn12 N14 2.1975(17) . . yes
```

```
Mn12 N15 2.1176(16) . . yes
```

```
Mn12 N16 2.2557(16) . . yes
```

```
P21 F21 1.6074(15) . . yes
```

```
P21 F22 1.6031(16) . . yes
```

```
P21 F23 1.6009(14) . . yes
```

```
P21 F24 1.6070(15) . . yes
```

```
P21 F25 1.5991(15) . . yes
```

```
P21 F26 1.5954(14) . . yes
```

```
P31 F31 1.620(2) . . yes
```

```
P31 F32 1.5824(17) . . yes
```

```
P31 F33 1.6029(18) . . yes
```

```
P31 F34 1.556(2) . . yes
```

```
P31 F35 1.5928(18) . . yes
```

```
P31 F36 1.5972(16) . . yes
```

```
O12 C11 1.266(2) . . yes
```

```
O13 C11 1.255(2) . . yes
```

```
O14 C18 1.259(2) . . yes
```

```
O15 C18 1.266(2) . . yes
```

```
N11 C115 1.476(3) . . yes
```

```
N11 C116 1.484(2) . . yes
```

```
N11 C123 1.491(3) . . yes
```

```
N12 C119 1.498(2) . . yes
```

```
N12 C117 1.507(3) . . yes
```

```
N12 C118 1.492(3) . . yes
```

N13	C122	1.488(3)	.	.	yes
N13	C121	1.479(3)	.	.	yes
N13	C120	1.496(3)	.	.	yes
N14	C125	1.495(2)	.	.	yes
N14	C132	1.484(3)	.	.	yes
N14	C124	1.479(3)	.	.	yes
N15	C126	1.491(2)	.	.	yes
N15	C127	1.489(3)	.	.	yes
N15	C128	1.505(2)	.	.	yes
N16	C130	1.470(3)	.	.	yes
N16	C131	1.493(3)	.	.	yes
N16	C129	1.483(3)	.	.	yes
C11	C12	1.497(2)	.	.	no
C12	C13	1.395(3)	.	.	no
C12	C17	1.399(3)	.	.	no
C13	C14	1.390(3)	.	.	no
C14	C15	1.384(3)	.	.	no
C15	C16	1.386(3)	.	.	no
C16	C17	1.390(3)	.	.	no
C18	C19	1.496(3)	.	.	no
C19	C110	1.388(3)	.	.	no
C19	C114	1.394(3)	.	.	no
C110	C111	1.393(3)	.	.	no
C111	C112	1.385(3)	.	.	no
C112	C113	1.383(3)	.	.	no
C113	C114	1.391(3)	.	.	no
C13	H13	0.9500	.	.	no
C14	H14	0.9499	.	.	no
C15	H15	0.9500	.	.	no
C16	H16	0.9499	.	.	no
C116	C117	1.517(3)	.	.	no
C17	H17	0.9500	.	.	no
C119	C120	1.512(3)	.	.	no
C122	C123	1.521(3)	.	.	no
C125	C126	1.513(3)	.	.	no
C128	C129	1.515(3)	.	.	no
C131	C132	1.524(3)	.	.	no
C110	H110	0.9500	.	.	no
C111	H111	0.9500	.	.	no
C112	H112	0.9500	.	.	no
C113	H113	0.9499	.	.	no
C114	H114	0.9501	.	.	no
C115	H115"	0.9800	.	.	no
C115	H115	0.9800	.	.	no
C115	H115'	0.9800	.	.	no
C116	H116'	0.9901	.	.	no
C116	H116	0.9899	.	.	no
C117	H117'	0.9901	.	.	no
C117	H117	0.9899	.	.	no
C118	H118	0.9799	.	.	no
C118	H118"	0.9800	.	.	no
C118	H118'	0.9801	.	.	no
C119	H119'	0.9900	.	.	no
C119	H119	0.9900	.	.	no
C120	H120	0.9899	.	.	no
C120	H120'	0.9900	.	.	no
C121	H121'	0.9803	.	.	no
C121	H121"	0.9798	.	.	no
C121	H121	0.9799	.	.	no
C122	H122'	0.9900	.	.	no
C122	H122	0.9900	.	.	no

C123 H123 0.9900 . . no
 C123 H123' 0.9900 . . no
 C124 H124 0.9800 . . no
 C124 H124" 0.9801 . . no
 C124 H124' 0.9800 . . no
 C125 H125 0.9900 . . no
 C125 H125' 0.9900 . . no
 C126 H126' 0.9900 . . no
 C126 H126 0.9900 . . no
 C127 H127' 0.9800 . . no
 C127 H127" 0.9800 . . no
 C127 H127 0.9800 . . no
 C128 H128 0.9900 . . no
 C128 H128' 0.9900 . . no
 C129 H129' 0.9900 . . no
 C129 H129 0.9899 . . no
 C130 H130' 0.9804 . . no
 C130 H130" 0.9800 . . no
 C130 H130 0.9796 . . no
 C131 H131' 0.9901 . . no
 C131 H131 0.9900 . . no
 C132 H132 0.9900 . . no
 C132 H132' 0.9901 . . no

loop_

_geom_angle_atom_site_label_1
 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
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 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_2
 _geom_angle_site_symmetry_3
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 O11 Mn11 O12 95.66(6) . . . yes
 O11 Mn11 O14 95.97(6) . . . yes
 O11 Mn11 N11 96.73(6) . . . yes
 O11 Mn11 N12 175.19(6) . . . yes
 O11 Mn11 N13 95.18(6) . . . yes
 O12 Mn11 O14 96.78(6) . . . yes
 O12 Mn11 N11 88.55(6) . . . yes
 O12 Mn11 N12 88.31(6) . . . yes
 O12 Mn11 N13 164.69(6) . . . yes
 O14 Mn11 N11 165.67(6) . . . yes
 O14 Mn11 N12 86.24(6) . . . yes
 O14 Mn11 N13 92.80(6) . . . yes
 N11 Mn11 N12 80.61(6) . . . yes
 N11 Mn11 N13 79.47(6) . . . yes
 N12 Mn11 N13 80.41(6) . . . yes
 O11 Mn12 O13 95.23(6) . . . yes
 O11 Mn12 O15 95.01(6) . . . yes
 O11 Mn12 N14 95.43(6) . . . yes
 O11 Mn12 N15 175.56(6) . . . yes
 O11 Mn12 N16 97.72(6) . . . yes
 O13 Mn12 O15 97.34(5) . . . yes
 O13 Mn12 N14 93.05(6) . . . yes
 O13 Mn12 N15 86.22(6) . . . yes
 O13 Mn12 N16 165.63(6) . . . yes
 O15 Mn12 N14 164.54(6) . . . yes
 O15 Mn12 N15 88.96(6) . . . yes
 O15 Mn12 N16 87.76(6) . . . yes
 N14 Mn12 N15 80.29(6) . . . yes

N14 Mn12 N16 79.56(6) . . . yes
 N15 Mn12 N16 80.42(6) . . . yes
 F25 P21 F26 90.21(8) . . . yes
 F21 P21 F22 90.26(8) . . . yes
 F21 P21 F23 89.58(7) . . . yes
 F21 P21 F24 179.34(7) . . . yes
 F21 P21 F25 90.32(8) . . . yes
 F21 P21 F26 90.17(8) . . . yes
 F22 P21 F23 89.50(8) . . . yes
 F22 P21 F24 89.88(8) . . . yes
 F22 P21 F25 179.27(8) . . . yes
 F22 P21 F26 90.24(8) . . . yes
 F23 P21 F24 89.78(7) . . . yes
 F23 P21 F25 90.06(7) . . . yes
 F23 P21 F26 179.63(7) . . . yes
 F24 P21 F25 89.54(7) . . . yes
 F24 P21 F26 90.48(8) . . . yes
 F35 P31 F36 89.16(10) . . . yes
 F31 P31 F32 87.61(12) . . . yes
 F31 P31 F33 91.65(11) . . . yes
 F31 P31 F34 178.37(11) . . . yes
 F31 P31 F35 87.73(12) . . . yes
 F31 P31 F36 88.31(10) . . . yes
 F32 P31 F33 90.10(10) . . . yes
 F32 P31 F34 93.12(13) . . . yes
 F32 P31 F35 175.12(13) . . . yes
 F32 P31 F36 89.25(10) . . . yes
 F33 P31 F34 89.81(11) . . . yes
 F33 P31 F35 91.49(10) . . . yes
 F33 P31 F36 179.35(9) . . . yes
 F34 P31 F35 91.50(13) . . . yes
 F34 P31 F36 90.24(10) . . . yes
 Mn11 O11 Mn12 121.78(8) . . . yes
 Mn11 O12 C11 128.43(12) . . . yes
 Mn12 O13 C11 129.76(12) . . . yes
 Mn11 O14 C18 130.14(13) . . . yes
 Mn12 O15 C18 129.11(12) . . . yes
 Mn11 N11 C116 102.73(12) . . . yes
 Mn11 N11 C123 110.00(12) . . . yes
 Mn11 N11 C115 111.82(12) . . . yes
 C115 N11 C123 109.94(16) . . . yes
 C116 N11 C123 112.65(15) . . . yes
 C115 N11 C116 109.56(15) . . . yes
 C117 N12 C118 109.37(15) . . . yes
 C117 N12 C119 110.23(15) . . . yes
 Mn11 N12 C117 111.90(12) . . . yes
 Mn11 N12 C118 111.85(12) . . . yes
 Mn11 N12 C119 104.93(11) . . . yes
 C118 N12 C119 108.43(16) . . . yes
 C120 N13 C122 112.44(17) . . . yes
 C121 N13 C122 109.85(16) . . . yes
 Mn11 N13 C120 109.89(12) . . . yes
 Mn11 N13 C121 111.92(13) . . . yes
 Mn11 N13 C122 103.33(11) . . . yes
 C120 N13 C121 109.33(16) . . . yes
 C125 N14 C132 112.51(15) . . . yes
 Mn12 N14 C132 103.90(11) . . . yes
 Mn12 N14 C124 111.30(12) . . . yes
 Mn12 N14 C125 110.15(12) . . . yes
 C124 N14 C125 108.97(15) . . . yes
 C124 N14 C132 109.97(16) . . . yes

C126	N15	C127	109.08(14)	. . .	yes
Mn12	N15	C128	112.20(11)	. . .	yes
Mn12	N15	C126	105.41(12)	. . .	yes
Mn12	N15	C127	110.81(11)	. . .	yes
C126	N15	C128	110.02(14)	. . .	yes
C127	N15	C128	109.24(15)	. . .	yes
C129	N16	C131	112.74(15)	. . .	yes
Mn12	N16	C129	102.52(12)	. . .	yes
Mn12	N16	C130	112.84(12)	. . .	yes
Mn12	N16	C131	109.36(11)	. . .	yes
C129	N16	C130	109.07(16)	. . .	yes
C130	N16	C131	110.15(17)	. . .	yes
O12	C11	C12	116.67(16)	. . .	yes
O12	C11	O13	124.98(16)	. . .	yes
O13	C11	C12	118.32(16)	. . .	yes
C13	C12	C17	119.66(17)	. . .	no
C11	C12	C13	120.53(16)	. . .	no
C11	C12	C17	119.72(16)	. . .	no
C12	C13	C14	119.81(18)	. . .	no
C13	C14	C15	120.17(19)	. . .	no
C14	C15	C16	120.46(18)	. . .	no
C15	C16	C17	119.84(19)	. . .	no
C12	C17	C16	120.03(18)	. . .	no
O15	C18	C19	117.04(16)	. . .	yes
O14	C18	O15	124.99(17)	. . .	yes
O14	C18	C19	117.96(16)	. . .	yes
C110	C19	C114	120.04(18)	. . .	no
C18	C19	C110	120.43(17)	. . .	no
C18	C19	C114	119.52(17)	. . .	no
C19	C110	C111	119.79(18)	. . .	no
C110	C111	C112	120.0(2)	. . .	no
C111	C112	C113	120.4(2)	. . .	no
C12	C13	H13	120.10	. . .	no
C112	C113	C114	119.91(19)	. . .	no
C14	C13	H13	120.09	. . .	no
C19	C114	C113	119.85(18)	. . .	no
C13	C14	H14	119.93	. . .	no
C15	C14	H14	119.90	. . .	no
C14	C15	H15	119.77	. . .	no
C16	C15	H15	119.77	. . .	no
C15	C16	H16	120.08	. . .	no
C17	C16	H16	120.08	. . .	no
N11	C116	C117	110.80(15)	. . .	yes
C16	C17	H17	119.98	. . .	no
N12	C117	C116	111.33(15)	. . .	yes
C12	C17	H17	119.99	. . .	no
N12	C119	C120	110.42(17)	. . .	yes
N13	C120	C119	109.56(16)	. . .	yes
N13	C122	C123	111.23(17)	. . .	yes
N11	C123	C122	110.70(17)	. . .	yes
N14	C125	C126	109.74(15)	. . .	yes
N15	C126	C125	110.02(15)	. . .	yes
N15	C128	C129	111.30(15)	. . .	yes
N16	C129	C128	110.66(16)	. . .	yes
N16	C131	C132	110.94(16)	. . .	yes
N14	C132	C131	111.06(18)	. . .	yes
C19	C110	H110	120.09	. . .	no
C111	C110	H110	120.11	. . .	no
C110	C111	H111	120.00	. . .	no
C112	C111	H111	120.01	. . .	no
C113	C112	H112	119.80	. . .	no

C111 C112 H112 119.80 . . . no
C112 C113 H113 120.04 . . . no
C114 C113 H113 120.05 . . . no
C113 C114 H114 120.08 . . . no
C19 C114 H114 120.07 . . . no
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H116' C116 H116 108.07 . . . no
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C126 C125 H125' 109.72 . . . no

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 C125 C126 H126' 109.65 . . . no
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 H127' C127 H127 109.48 . . . no
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 N15 C128 H128' 109.37 . . . no
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 C128 C129 H129' 109.51 . . . no
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 N16 C130 H130' 109.45 . . . no
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 H130' C130 H130" 109.43 . . . no
 H130' C130 H130 109.47 . . . no
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 C132 C131 H131 109.46 . . . no
 N16 C131 H131 109.45 . . . no
 C132 C131 H131' 109.45 . . . no
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 H132' C132 H132 108.02 . . . no
 N14 C132 H132' 109.42 . . . no
 N14 C132 H132 109.43 . . . no
 C131 C132 H132' 109.43 . . . no
 C131 C132 H132 109.43 . . . no

loop_

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 O14 Mn11 O11 Mn12 43.34(9) . . . . no
 N11 Mn11 O11 Mn12 -143.32(8) . . . . no
 N13 Mn11 O11 Mn12 136.71(8) . . . . no
 O11 Mn11 O12 C11 28.88(17) . . . . no
 O14 Mn11 O12 C11 -67.83(17) . . . . no
 N11 Mn11 O12 C11 125.51(17) . . . . no
 N12 Mn11 O12 C11 -153.85(17) . . . . no
 O11 Mn11 O14 C18 -2.85(15) . . . . no

O12	Mn11	O14	C18	93.59(15)	. . . .	no
N12	Mn11	O14	C18	-178.56(15)	. . . .	no
N13	Mn11	O14	C18	-98.36(15)	. . . .	no
O11	Mn11	N11	C115	35.65(13)	. . . .	no
O11	Mn11	N11	C116	153.04(11)	. . . .	no
O11	Mn11	N11	C123	-86.80(12)	. . . .	no
O12	Mn11	N11	C115	-59.88(13)	. . . .	no
O12	Mn11	N11	C116	57.52(11)	. . . .	no
O12	Mn11	N11	C123	177.67(12)	. . . .	no
N12	Mn11	N11	C115	-148.41(13)	. . . .	no
N12	Mn11	N11	C116	-31.01(11)	. . . .	no
N12	Mn11	N11	C123	89.14(13)	. . . .	no
N13	Mn11	N11	C115	129.69(13)	. . . .	no
N13	Mn11	N11	C116	-112.91(11)	. . . .	no
N13	Mn11	N11	C123	7.24(12)	. . . .	no
O12	Mn11	N12	C117	-81.24(12)	. . . .	no
O12	Mn11	N12	C118	41.88(13)	. . . .	no
O12	Mn11	N12	C119	159.22(13)	. . . .	no
O14	Mn11	N12	C117	-178.16(12)	. . . .	no
O14	Mn11	N12	C118	-55.04(13)	. . . .	no
O14	Mn11	N12	C119	62.31(12)	. . . .	no
N11	Mn11	N12	C117	7.56(12)	. . . .	no
N11	Mn11	N12	C118	130.68(13)	. . . .	no
N11	Mn11	N12	C119	-111.97(13)	. . . .	no
N13	Mn11	N12	C117	88.36(12)	. . . .	no
N13	Mn11	N12	C118	-148.52(14)	. . . .	no
N13	Mn11	N12	C119	-31.17(13)	. . . .	no
O11	Mn11	N13	C120	-175.79(14)	. . . .	no
O11	Mn11	N13	C121	-54.12(15)	. . . .	no
O11	Mn11	N13	C122	64.02(12)	. . . .	no
O14	Mn11	N13	C120	-79.54(14)	. . . .	no
O14	Mn11	N13	C121	42.13(14)	. . . .	no
O14	Mn11	N13	C122	160.27(12)	. . . .	no
N11	Mn11	N13	C120	88.30(14)	. . . .	no
N11	Mn11	N13	C121	-150.02(15)	. . . .	no
N11	Mn11	N13	C122	-31.89(12)	. . . .	no
N12	Mn11	N13	C120	6.17(13)	. . . .	no
N12	Mn11	N13	C121	127.85(15)	. . . .	no
N12	Mn11	N13	C122	-114.02(12)	. . . .	no
O13	Mn12	O11	Mn11	43.89(9)	. . . .	no
O15	Mn12	O11	Mn11	-53.97(8)	. . . .	no
N14	Mn12	O11	Mn11	137.46(8)	. . . .	no
N16	Mn12	O11	Mn11	-142.37(8)	. . . .	no
O11	Mn12	O13	C11	-0.10(17)	. . . .	no
O15	Mn12	O13	C11	95.65(17)	. . . .	no
N14	Mn12	O13	C11	-95.83(17)	. . . .	no
N15	Mn12	O13	C11	-175.89(17)	. . . .	no
O11	Mn12	O15	C18	34.15(16)	. . . .	no
O13	Mn12	O15	C18	-61.79(16)	. . . .	no
N15	Mn12	O15	C18	-147.84(16)	. . . .	no
N16	Mn12	O15	C18	131.71(16)	. . . .	no
O11	Mn12	N14	C124	-53.43(13)	. . . .	no
O11	Mn12	N14	C125	-174.40(11)	. . . .	no
O11	Mn12	N14	C132	64.88(12)	. . . .	no
O13	Mn12	N14	C124	42.12(13)	. . . .	no
O13	Mn12	N14	C125	-78.85(12)	. . . .	no
O13	Mn12	N14	C132	160.42(12)	. . . .	no
N15	Mn12	N14	C124	127.76(13)	. . . .	no
N15	Mn12	N14	C125	6.79(11)	. . . .	no
N15	Mn12	N14	C132	-113.94(12)	. . . .	no
N16	Mn12	N14	C124	-150.30(14)	. . . .	no

N16	Mn12	N14	C125	88.73(12)	. . . .	no
N16	Mn12	N14	C132	-32.00(12)	. . . .	no
O13	Mn12	N15	C126	62.10(11)	. . . .	no
O13	Mn12	N15	C127	-55.77(12)	. . . .	no
O13	Mn12	N15	C128	-178.17(13)	. . . .	no
O15	Mn12	N15	C126	159.53(11)	. . . .	no
O15	Mn12	N15	C127	41.66(12)	. . . .	no
O15	Mn12	N15	C128	-80.75(13)	. . . .	no
N14	Mn12	N15	C126	-31.64(11)	. . . .	no
N14	Mn12	N15	C127	-149.51(12)	. . . .	no
N14	Mn12	N15	C128	88.09(13)	. . . .	no
N16	Mn12	N15	C126	-112.58(12)	. . . .	no
N16	Mn12	N15	C127	129.56(12)	. . . .	no
N16	Mn12	N15	C128	7.15(12)	. . . .	no
O11	Mn12	N16	C129	153.23(11)	. . . .	no
O11	Mn12	N16	C130	36.05(15)	. . . .	no
O11	Mn12	N16	C131	-86.92(13)	. . . .	no
O15	Mn12	N16	C129	58.48(11)	. . . .	no
O15	Mn12	N16	C130	-58.70(15)	. . . .	no
O15	Mn12	N16	C131	178.33(13)	. . . .	no
N14	Mn12	N16	C129	-112.64(12)	. . . .	no
N14	Mn12	N16	C130	130.18(15)	. . . .	no
N14	Mn12	N16	C131	7.21(12)	. . . .	no
N15	Mn12	N16	C129	-30.85(11)	. . . .	no
N15	Mn12	N16	C130	-148.02(15)	. . . .	no
N15	Mn12	N16	C131	89.00(13)	. . . .	no
Mn11	O12	C11	O13	7.6(3)	. . . .	no
Mn11	O12	C11	C12	-170.13(13)	. . . .	no
Mn12	O13	C11	O12	-25.0(3)	. . . .	no
Mn12	O13	C11	C12	152.71(14)	. . . .	no
Mn11	O14	C18	O15	-16.9(3)	. . . .	no
Mn11	O14	C18	C19	162.39(12)	. . . .	no
Mn12	O15	C18	O14	-2.0(3)	. . . .	no
Mn12	O15	C18	C19	178.75(12)	. . . .	no
Mn11	N11	C116	C117	50.28(16)	. . . .	no
C115	N11	C116	C117	169.27(16)	. . . .	no
C123	N11	C116	C117	-68.0(2)	. . . .	no
Mn11	N11	C123	C122	19.30(19)	. . . .	no
C115	N11	C123	C122	-104.26(19)	. . . .	no
C116	N11	C123	C122	133.25(18)	. . . .	no
Mn11	N12	C117	C116	17.79(18)	. . . .	no
C118	N12	C117	C116	-106.72(17)	. . . .	no
C119	N12	C117	C116	134.16(16)	. . . .	no
Mn11	N12	C119	C120	53.51(17)	. . . .	no
C117	N12	C119	C120	-67.14(19)	. . . .	no
C118	N12	C119	C120	173.16(16)	. . . .	no
Mn11	N13	C120	C119	20.60(19)	. . . .	no
C121	N13	C120	C119	-102.61(19)	. . . .	no
C122	N13	C120	C119	135.10(17)	. . . .	no
Mn11	N13	C122	C123	53.93(17)	. . . .	no
C120	N13	C122	C123	-64.5(2)	. . . .	no
C121	N13	C122	C123	173.49(16)	. . . .	no
Mn12	N14	C125	C126	19.73(17)	. . . .	no
C124	N14	C125	C126	-102.63(18)	. . . .	no
C132	N14	C125	C126	135.14(16)	. . . .	no
Mn12	N14	C132	C131	53.94(16)	. . . .	no
C124	N14	C132	C131	173.16(16)	. . . .	no
C125	N14	C132	C131	-65.2(2)	. . . .	no
Mn12	N15	C126	C125	53.21(15)	. . . .	no
C127	N15	C126	C125	172.24(15)	. . . .	no
C128	N15	C126	C125	-67.95(19)	. . . .	no

Mn12 N15 C128 C129 18.4(2) . . . . no
C126 N15 C128 C129 135.43(17) . . . . no
C127 N15 C128 C129 -104.86(18) . . . . no
Mn12 N16 C129 C128 50.37(16) . . . . no
C130 N16 C129 C128 170.20(16) . . . . no
C131 N16 C129 C128 -67.1(2) . . . . no
Mn12 N16 C131 C132 19.29(19) . . . . no
C129 N16 C131 C132 132.64(17) . . . . no
C130 N16 C131 C132 -105.27(19) . . . . no
O13 C11 C12 C17 -171.63(19) . . . . no
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C11 C12 C13 C14 -175.1(2) . . . . no
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