Supplementary data for

Synthesis of Mn-MOFs loaded zinc phosphate composite to water-based acrylic coating with durable anticorrosion performance on mild steel

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c School of Life and Environmental Sciences, Guilin University of Electronic Technology, Guilin,541004,P.R.China)

The CIF structure file data of complex Mn-MOFs

data_19101309-1

_audit_creation_date 2020-02-04

_audit_creation_method

;

Olex2 1.2-beta

(compiled 2018.05.29 svn.r3508 for OlexSys, GUI svn.r5506)

;

_shelxl_version_number 2013-2

_audit_contact_author_address ?

_audit_contact_author_email ?

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_audit_contact_author_name ''

_audit_contact_author_phone ?

_publ_contact_author_id_orcid ?

_publ_section_references

;

Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H.

(2009), J. Appl. Cryst. 42, 339-341.

Sheldrick, G.M. (2015). Acta Cryst. C71, 3-8.

;

_chemical_name_common ?

_chemical_name_systematic

;

?

;

_chemical_formula_moiety 'C20 H12 Mn N2 O5'

_chemical_formula_sum 'C20 H12 Mn N2 O5'

_chemical_formula_weight 415.26

_chemical_absolute_configuration ?

_chemical_melting_point ?

loop_

_atom_type_symbol

_atom_type_description

_atom_type_scat_dispersion_real

_atom_type_scat_dispersion_imag

_atom_type_scat_source

'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'

'Mn' 'Mn' 0.3368 0.7283 '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'

_shelx_space_group_comment

;

The symmetry employed for this shelxl refinement is uniquely defined

by the following loop, which should always be used as a source of

symmetry information in preference to the above space-group names.

They are only intended as comments.

;

_space_group_crystal_system 'orthorhombic'

_space_group_IT_number 19

_space_group_name_H-M_alt 'P 21 21 21'

_space_group_name_Hall 'P 2ac 2ab'

loop_

_space_group_symop_operation_xyz

'x, y, z'

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

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

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

_cell_length_a 4.8722(2)

_cell_length_b 16.6989(6)

_cell_length_c 19.3540(6)

_cell_angle_alpha 90

_cell_angle_beta 90

_cell_angle_gamma 90

_cell_volume 1574.65(10)

_cell_formula_units_Z 4

_cell_measurement_reflns_used 2826

_cell_measurement_temperature 293(2)

_cell_measurement_theta_max 26.7510

_cell_measurement_theta_min 3.7960

_shelx_estimated_absorpt_T_max ?

_shelx_estimated_absorpt_T_min ?

_exptl_absorpt_coefficient_mu 0.879

_exptl_absorpt_correction_T_max 1.00000

_exptl_absorpt_correction_T_min 0.32629

_exptl_absorpt_correction_type multi-scan

_exptl_absorpt_process_details

;

CrysAlisPro 1.171.39.46 (Rigaku Oxford Diffraction, 2018)

Empirical absorption correction using spherical harmonics,

implemented in SCALE3 ABSPACK scaling algorithm.

;

_exptl_crystal_colour yellow

_exptl_crystal_density_diffrn 1.752

_exptl_crystal_density_meas ?

_exptl_crystal_density_method ?

_exptl_crystal_description bolck

_exptl_crystal_F_000 844

_exptl_crystal_size_max 0.33

_exptl_crystal_size_mid 0.26

_exptl_crystal_size_min 0.21

_exptl_special_details

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_exptl_transmission_factor_max ?

_exptl_transmission_factor_min ?

_diffrn_reflns_av_R_equivalents 0.0600

_diffrn_reflns_av_unetI/netI 0.0748

_diffrn_reflns_Laue_measured_fraction_full 0.996

_diffrn_reflns_Laue_measured_fraction_max 0.914

_diffrn_reflns_limit_h_max 6

_diffrn_reflns_limit_h_min -6

_diffrn_reflns_limit_k_max 16

_diffrn_reflns_limit_k_min -21

_diffrn_reflns_limit_l_max 24

_diffrn_reflns_limit_l_min -26

_diffrn_reflns_number 11654

_diffrn_reflns_point_group_measured_fraction_full 0.998

_diffrn_reflns_point_group_measured_fraction_max 0.878

_diffrn_reflns_theta_full 25.242

_diffrn_reflns_theta_max 29.162

_diffrn_reflns_theta_min 3.385

_diffrn_ambient_temperature 293(2)

_diffrn_detector_area_resol_mean ?

_diffrn_measured_fraction_theta_full 0.996

_diffrn_measured_fraction_theta_max 0.914

_diffrn_measurement_device_type 'multiwire proportional'

_diffrn_measurement_method 'phi and omega scans'

_diffrn_radiation_monochromator 'graphite'

_diffrn_radiation_type MoK\a

_diffrn_radiation_wavelength 0.71073

_diffrn_source ?

_reflns_Friedel_coverage 0.648

_reflns_Friedel_fraction_full 1.000

_reflns_Friedel_fraction_max 0.827

_reflns_number_gt 3026

_reflns_number_total 3741

_reflns_special_details

;

Reflections were merged by SHELXL according to the crystal class for the calculation of statistics and refinement.

_reflns_Friedel_fraction is defined as the number of unique Friedel pairs measured divided by the number that would be possible theoretically, ignoring centric projections and systematic absences.

;

_reflns_threshold_expression 'I > 2\s(I)'

_computing_cell_refinement ?

_computing_data_collection ?

_computing_data_reduction ?

_computing_molecular_graphics 'Olex2 (Dolomanov et al., 2009)'

_computing_publication_material 'Olex2 (Dolomanov et al., 2009)'

_computing_structure_refinement 'ShelXL (Sheldrick, 2015)'

_computing_structure_solution 'ShelXS (Sheldrick, 2008)'

_refine_diff_density_max 0.331

_refine_diff_density_min -0.430

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_refine_diff_density_rms          0.077
_refine_ls_abs_structure_details
;
 Flack x determined using 1047 quotients [(I+)-(I-)]/[(I+)+(I-)]
 (Parsons and Flack (2004), Acta Cryst. A60, s61).
;
_refine_ls_abs_structure_Flack     -0.018(17)
_refine_ls_extinction_coef         .
_refine_ls_extinction_method       none
_refine_ls_goodness_of_fit_ref     1.035
_refine_ls_hydrogen_treatment      mixed
_refine_ls_matrix_type             full
_refine_ls_number_parameters       258
_refine_ls_number_reflns           3741
_refine_ls_number_restraints       0
_refine_ls_R_factor_all            0.0643
_refine_ls_R_factor_gt             0.0435
_refine_ls_restrained_S_all        1.035
_refine_ls_shift/su_max            0.000
_refine_ls_shift/su_mean           0.000
_refine_ls_structure_factor_coef   Fsqd
_refine_ls_weighting_details
;
 w=1/[\s^2^(Fo^2^)+(0.0308P)^2^]
 where P=(Fo^2^+2Fc^2^)/3
;
_refine_ls_weighting_scheme        calc
_refine_ls_wR_factor_gt            0.0795
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_refine_ls_wR_factor_ref 0.0883

_refine_special_details

;

?

;

_olex2_refinement_description

;

1. Fixed Uiso

At 1.2 times of:

All C(H) groups

At 1.5 times of:

All O(H) groups

2.a Rotating group:

O5(H5A)

2.b Aromatic/amide H refined with riding coordinates:

C5(H5), C14(H14), C8(H8), C2(H2), C3(H3), C11(H11), C17(H17), C16(H16),

C4(H4), C15(H15)

;

_atom_sites_solution_hydrogens mixed

_atom_sites_solution_primary ?

_atom_sites_solution_secondary ?

loop_

_atom_site_label

_atom_site_type_symbol

_atom_site_fract_x

_atom_site_fract_y

_atom_site_fract_z

_atom_site_U_iso_or_equiv

_atom_site_adp_type

_atom_site_occupancy

_atom_site_site_symmetry_order

_atom_site_calc_flag

_atom_site_refinement_flags_posn

_atom_site_refinement_flags_adp

_atom_site_refinement_flags_occupancy

_atom_site_disorder_assembly

_atom_site_disorder_group

Mn1 Mn 0.04438(13) 0.69435(4) 0.05364(3) 0.01853(16) Uani 1 1 d . . . . .

O1 O -0.1266(5) 0.80760(17) 0.02376(13) 0.0188(6) Uani 1 1 d . . . . .

C6 C -0.0099(8) 1.0220(2) 0.05518(19) 0.0186(9) Uani 1 1 d . . . . .

C5 C 0.1916(9) 1.0468(3) 0.0073(2) 0.0239(10) Uani 1 1 d . . . . .

H5 H 0.2738 1.0090 -0.0213 0.029 Uiso 1 1 calc R . . . .

N5 N -0.3308(7) 1.0640(2) 0.14681(17) 0.0227(8) Uani 1 1 d . . . . .

N6 N -0.7449(8) 0.9007(2) 0.20659(16) 0.0215(8) Uani 1 1 d . . . . .

C13 C -1.0294(9) 0.9437(2) 0.30539(19) 0.0203(9) Uani 1 1 d . . . . .

C18 C -0.9444(9) 0.8862(2) 0.25455(18) 0.0188(9) Uani 1 1 d . . . . .

C14 C -1.2405(10) 0.9211(3) 0.3515(2) 0.0270(10) Uani 1 1 d . . . . .

H14 H -1.2984 0.9572 0.3851 0.032 Uiso 1 1 calc R . . . .

C8 C -0.3046(9) 0.9270(2) 0.11199(19) 0.0186(9) Uani 1 1 d . . . . .

H8 H -0.3702 0.8751 0.1174 0.022 Uiso 1 1 calc R . . . .

C20 C 0.0238(9) 0.8710(2) 0.02919(17) 0.0177(9) Uani 1 1 d . . . . .

C2 C -0.0525(10) 1.1619(2) 0.0917(2) 0.0308(11) Uani 1 1 d . . . . .

H2 H -0.1337 1.2008 0.1193 0.037 Uiso 1 1 calc R . . . .

C9 C -0.4141(9) 0.9891(2) 0.15300(19) 0.0195(9) Uani 1 1 d . . . . .

C7 C -0.1039(8) 0.9420(2) 0.06455(19) 0.0174(9) Uani 1 1 d . . . . .

C1 C -0.1342(9) 1.0811(3) 0.0985(2) 0.0232(10) Uani 1 1 d . . . . .

C3 C 0.1442(9) 1.1835(3) 0.0450(2) 0.0313(11) Uani 1 1 d . . . . .

H3 H 0.1969 1.2368 0.0412 0.038 Uiso 1 1 calc R . . . .

C11 C -0.6977(9) 1.0333(3) 0.2543(2) 0.0233(10) Uani 1 1 d . . . . .

H11 H -0.6104 1.0828 0.2524 0.028 Uiso 1 1 calc R . . . .

C17 C -1.0725(9) 0.8100(3) 0.2532(2) 0.0280(10) Uani 1 1 d . . . . .

H17 H -1.0151 0.7720 0.2212 0.034 Uiso 1 1 calc R . . . .

C10 C -0.6257(9) 0.9725(3) 0.2059(2) 0.0201(9) Uani 1 1 d . . . . .

C16 C -1.2789(10) 0.7916(3) 0.2982(2) 0.0305(11) Uani 1 1 d . . . . .

H16 H -1.3648 0.7420 0.2958 0.037 Uiso 1 1 calc R . . . .

C12 C -0.8932(9) 1.0199(2) 0.30357(19) 0.0207(10) Uani 1 1 d . . . . .

C4 C 0.2678(10) 1.1252(3) 0.0024(2) 0.0285(11) Uani 1 1 d . . . . .

H4 H 0.4019 1.1403 -0.0293 0.034 Uiso 1 1 calc R . . . .

C15 C -1.3612(9) 0.8475(3) 0.3478(2) 0.0289(11) Uani 1 1 d . . . . .

H15 H -1.5000 0.8343 0.3788 0.035 Uiso 1 1 calc R . . . .

O2 O 0.2651(6) 0.87390(17) 0.00940(14) 0.0254(7) Uani 1 1 d . . . . .

C19 C -0.9527(9) 1.0865(2) 0.35409(19) 0.0209(9) Uani 1 1 d . . . . .

O4 O -1.1453(6) 1.08036(18) 0.39683(14) 0.0282(7) Uani 1 1 d . . . . .

O3 O -0.8011(6) 1.14883(18) 0.35286(15) 0.0276(7) Uani 1 1 d . . . . .

O5 O 0.3385(7) 0.7485(2) 0.12709(16) 0.0303(8) Uani 1 1 d . . . . .

H5A H 0.4592 0.7133 0.1393 0.046 Uiso 1 1 d GR . . . .

H5B H 0.342(13) 0.791(4) 0.151(3) 0.10(3) Uiso 1 1 d . . . . .

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

Mn1 0.0211(3) 0.0145(3) 0.0199(3) 0.0018(3) 0.0000(3) -0.0010(3)

O1 0.0205(15) 0.0130(13) 0.0231(13) -0.0028(13) -0.0011(12) -0.0004(13)

C6 0.021(2) 0.0155(18) 0.0193(17) -0.0017(17) -0.003(2) -0.0021(16)

C5 0.029(3) 0.022(2) 0.021(2) -0.0029(18) 0.002(2) 0.0005(19)

N5 0.027(2) 0.019(2) 0.0221(17) -0.0027(15) 0.0043(17) 0.0014(16)

N6 0.025(2) 0.022(2) 0.0172(17) -0.0033(15) 0.0018(16) 0.0008(16)

C13 0.023(2) 0.020(2) 0.0179(18) -0.0002(16) -0.0040(19) 0.0028(19)

C18 0.021(2) 0.021(2) 0.0140(17) -0.0012(16) -0.0027(19) -0.0021(19)

C14 0.030(3) 0.028(3) 0.022(2) 0.0000(19) 0.004(2) 0.001(2)

C8 0.022(2) 0.016(2) 0.0185(19) -0.0017(17) -0.0013(18) 0.0011(17)

C20 0.025(2) 0.0148(19) 0.0132(17) 0.0008(15) -0.0007(18) 0.0036(19)

C2 0.037(3) 0.016(2) 0.039(2) -0.0063(19) 0.007(2) 0.001(2)

C9 0.020(2) 0.022(2) 0.0162(19) -0.0051(17) -0.0009(19) 0.0011(18)

C7 0.017(2) 0.018(2) 0.0174(19) -0.0021(16) -0.0018(18) -0.0006(16)

C1 0.026(3) 0.020(2) 0.024(2) -0.0029(19) -0.0024(19) 0.0025(19)

C3 0.037(3) 0.014(2) 0.042(3) 0.000(2) 0.000(2) -0.0052(19)

C11 0.026(3) 0.020(2) 0.024(2) -0.0029(18) 0.001(2) 0.0026(19)

C17 0.032(3) 0.023(2) 0.029(2) -0.007(2) 0.002(2) -0.002(2)

C10 0.023(2) 0.021(2) 0.017(2) -0.0027(17) 0.0020(19) 0.0026(18)

C16 0.038(3) 0.022(3) 0.031(2) -0.002(2) 0.001(2) -0.009(2)

C12 0.025(3) 0.021(2) 0.0162(19) -0.0041(17) 0.0000(19) 0.0034(18)

C4 0.032(3) 0.025(2) 0.029(2) 0.005(2) 0.007(2) -0.006(2)

C15 0.030(3) 0.032(3) 0.024(2) 0.000(2) 0.005(2) -0.001(2)

O2 0.0254(18) 0.0187(16) 0.0321(16) -0.0031(14) 0.0067(15) 0.0004(13)

C19 0.022(2) 0.021(2) 0.0202(19) -0.0033(17) -0.004(2) 0.005(2)

O4 0.0317(19) 0.0259(17) 0.0272(16) -0.0090(14) 0.0065(15) -0.0017(15)

O3 0.0326(19) 0.0218(17) 0.0285(16) -0.0067(14) 0.0082(15) -0.0002(14)

O5 0.029(2) 0.031(2) 0.0312(18) -0.0077(16) -0.0054(15) 0.0001(15)

_geom_special_details

;

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_

_geom_bond_atom_site_label_1

_geom_bond_atom_site_label_2

_geom_bond_distance

_geom_bond_site_symmetry_2

_geom_bond_publ_flag

Mn1 O1 2.146(3) . ?

Mn1 O1 2.194(3) 3_565 ?

Mn1 O2 2.154(3) 3_465 ?

Mn1 C19 2.575(4) 4_445 ?

Mn1 O4 2.187(3) 4_445 ?

Mn1 O3 2.293(3) 4_445 ?

Mn1 O5 2.212(3) . ?

O1 Mn1 2.194(3) 3_465 ?

O1 C20 1.292(5) . ?

C6 C5 1.412(6) . ?

C6 C7 1.424(5) . ?

C6 C1 1.429(5) . ?

C5 C4 1.364(6) . ?

N5 C9 1.322(5) . ?

N5 C1 1.368(5) . ?

N6 C18 1.366(5) . ?

N6 C10 1.332(5) . ?

C13 C18 1.435(5) . ?

C13 C14 1.413(6) . ?

C13 C12 1.436(6) . ?

C18 C17 1.418(6) . ?

C14 C15 1.364(6) . ?

C8 C9 1.410(5) . ?

C8 C7 1.365(5) . ?

C20 C7 1.504(5) . ?

C20 O2 1.237(5) . ?

C2 C1 1.413(6) . ?

C2 C3 1.366(6) . ?

C9 C10 1.479(5) . ?

C3 C4 1.411(6) . ?

C11 C10 1.425(5) . ?

C11 C12 1.366(6) . ?

C17 C16 1.364(6) . ?

C16 C15 1.398(6) . ?

C12 C19 1.509(5) . ?

O2 Mn1 2.154(3) 3_565 ?

C19 Mn1 2.575(4) 4_455 ?

C19 O4 1.255(5) . ?

C19 O3 1.277(5) . ?

O4 Mn1 2.187(3) 4_455 ?

O3 Mn1 2.293(3) 4_455 ?

loop_

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_geom_angle_atom_site_label_2

_geom_angle_atom_site_label_3

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O1 Mn1 O1 96.47(7) . 3_565 ?

O1 Mn1 O2 93.92(11) . 3_465 ?

O1 Mn1 C19 137.38(12) . 4_445 ?

O1 Mn1 C19 126.13(13) 3_565 4_445 ?

O1 Mn1 O4 166.49(10) . 4_445 ?

O1 Mn1 O3 155.72(11) 3_565 4_445 ?

O1 Mn1 O3 107.71(10) . 4_445 ?

O1 Mn1 O5 88.37(12) 3_565 . ?

O1 Mn1 O5 93.68(12) . . ?

O2 Mn1 O1 93.84(10) 3_465 3_565 ?

O2 Mn1 C19 85.02(12) 3_465 4_445 ?

O2 Mn1 O4 85.97(11) 3_465 4_445 ?

O2 Mn1 O3 86.85(11) 3_465 4_445 ?

O2 Mn1 O5 171.80(12) 3_465 . ?

O4 Mn1 O1 97.01(11) 4_445 3_565 ?

O4 Mn1 C19 29.12(12) 4_445 4_445 ?

O4 Mn1 O3 58.79(11) 4_445 4_445 ?

O4 Mn1 O5 85.92(12) 4_445 . ?

O3 Mn1 C19 29.69(12) 4_445 4_445 ?

O5 Mn1 C19 87.30(13) . 4_445 ?

O5 Mn1 O3 87.90(12) . 4_445 ?

Mn1 O1 Mn1 117.03(12) . 3_465 ?

C20 O1 Mn1 118.8(2) . 3_465 ?

C20 O1 Mn1 118.7(2) . . ?

C5 C6 C7 125.6(4) . . ?

C5 C6 C1 118.5(4) . . ?

C7 C6 C1 115.9(4) . . ?

C4 C5 C6 121.1(4) . . ?

C9 N5 C1 118.3(3) . . ?

C10 N6 C18 118.4(4) . . ?

C18 C13 C12 116.2(4) . . ?

C14 C13 C18 117.7(4) . . ?

C14 C13 C12 126.0(4) . . ?

N6 C18 C13 123.6(4) . . ?

N6 C18 C17 117.4(4) . . ?

C17 C18 C13 119.0(4) . . ?

C15 C14 C13 121.4(4) . . ?

C7 C8 C9 121.0(4) . . ?

O1 C20 C7 116.6(4) . . ?

O2 C20 O1 123.1(4) . . ?

O2 C20 C7 120.2(4) . . ?

C3 C2 C1 120.8(4) . . ?

N5 C9 C8 121.9(4) . . ?

N5 C9 C10 117.0(4) . . ?

C8 C9 C10 121.1(4) . . ?

C6 C7 C20 123.3(4) . . ?

C8 C7 C6 119.2(4) . . ?

C8 C7 C20 117.3(4) . . ?

N5 C1 C6 123.7(4) . . ?

N5 C1 C2 117.4(4) . . ?

C2 C1 C6 119.0(4) . . ?

C2 C3 C4 120.3(4) . . ?

C12 C11 C10 120.9(4) . . ?

C16 C17 C18 121.0(4) . . ?

N6 C10 C9 118.6(4) . . ?

N6 C10 C11 121.8(4) . . ?

C11 C10 C9 119.6(4) . . ?

C17 C16 C15 120.0(4) . . ?

C13 C12 C19 123.3(4) . . ?

C11 C12 C13 119.0(4) . . ?

C11 C12 C19 117.7(4) . . ?

C5 C4 C3 120.3(4) . . ?

C14 C15 C16 120.9(4) . . ?

C20 O2 Mn1 139.0(3) . 3_565 ?

C12 C19 Mn1 176.4(3) . 4_455 ?

O4 C19 Mn1 58.0(2) . 4_455 ?

O4 C19 C12 120.7(4) . . ?

O4 C19 O3 120.7(4) . . ?

O3 C19 Mn1 62.8(2) . 4_455 ?

O3 C19 C12 118.5(4) . . ?

C19 O4 Mn1 92.9(2) . 4_455 ?

C19 O3 Mn1 87.5(2) . 4_455 ?

```
loop_
 _refln_index_h
 _refln_index_k
 _refln_index_l
 _refln_F_squared_meas
 _refln_F_squared_sigma

_iucr_refine_instructions_details
;
TITL 19101309-1 in P212121 #19
REM reset to P212121 #19
CELL 0.71073 4.8722 16.6989 19.354 90 90 90
ZERR 4 0.0002 0.0006 0.0006 0 0 0
LATT -1
SYMM 0.5-X,-Y,0.5+Z
SYMM 0.5+X,0.5-Y,-Z
SYMM -X,0.5+Y,0.5-Z
SFAC C H Mn N O
UNIT 80 48 4 8 20

L.S. 99
PLAN  20
BOND
fmap 2 53
acta
REM <olex2.extras>
REM <HklSrc "%.\\19101309-1.hkl">
```

REM </olex2.extras>

WGHT 0.030800

FVAR 0.41391

MN1 3 0.044377 0.694346 0.053642 11.00000 0.02114 0.01450 =
0.01994 0.00181 -0.00003 -0.00100

O1 5 -0.126636 0.807602 0.023764 11.00000 0.02049 0.01300 =
0.02305 -0.00280 -0.00114 -0.00036

C6 1 -0.009927 1.022003 0.055179 11.00000 0.02103 0.01553 =
0.01929 -0.00169 -0.00344 -0.00206

C5 1 0.191633 1.046755 0.007286 11.00000 0.02912 0.02156 =
0.02111 -0.00291 0.00236 0.00051

AFIX 43

H5 2 0.273774 1.008995 -0.021350 11.00000 -1.20000

AFIX 0

N5 4 -0.330794 1.064035 0.146807 11.00000 0.02675 0.01941 =
0.02208 -0.00267 0.00434 0.00138

N6 4 -0.744868 0.900699 0.206592 11.00000 0.02520 0.02206 =
0.01722 -0.00334 0.00184 0.00084

C13 1 -1.029429 0.943652 0.305386 11.00000 0.02262 0.02035 =
0.01789 -0.00019 -0.00399 0.00278

C18 1 -0.944352 0.886207 0.254549 11.00000 0.02105 0.02142 =
0.01404 -0.00123 -0.00270 -0.00212

C14 1 -1.240488 0.921073 0.351496 11.00000 0.03031 0.02837 =
0.02231 0.00003 0.00404 0.00109

AFIX 43

H14 2 -1.298377 0.957152 0.385076 11.00000 -1.20000

AFIX 0

C8 1 -0.304614 0.927034 0.111993 11.00000 0.02179 0.01558 =
0.01849 -0.00174 -0.00133 0.00108

AFIX 43

H8 2 -0.370214 0.875105 0.117353 11.00000 -1.20000

AFIX 0

C20 1 0.023801 0.870991 0.029186 11.00000 0.02501 0.01481 =
0.01322 0.00077 -0.00072 0.00355

C2 1 -0.052524 1.161855 0.091679 11.00000 0.03724 0.01645 =
0.03881 -0.00634 0.00738 0.00137

AFIX 43

H2 2 -0.133660 1.200792 0.119304 11.00000 -1.20000

AFIX 0

C9 1 -0.414096 0.989058 0.153004 11.00000 0.02023 0.02195 =
0.01617 -0.00513 -0.00085 0.00106

C7 1 -0.103853 0.942010 0.064546 11.00000 0.01697 0.01796 =
0.01738 -0.00208 -0.00175 -0.00061

C1 1 -0.134181 1.081052 0.098515 11.00000 0.02580 0.02013 =
0.02380 -0.00289 -0.00236 0.00252

C3 1 0.144238 1.183453 0.044961 11.00000 0.03749 0.01442 =
0.04187 0.00012 -0.00011 -0.00519

AFIX 43

H3 2 0.196931 1.236807 0.041239 11.00000 -1.20000

AFIX 0

C11 1 -0.697685 1.033282 0.254346 11.00000 0.02605 0.02024 =
0.02353 -0.00287 0.00142 0.00265

AFIX 43

H11 2 -0.610354 1.082752 0.252388 11.00000 -1.20000

AFIX 0

C17 1 -1.072541 0.809984 0.253206 11.00000 0.03235 0.02304 =
0.02857 -0.00689 0.00197 -0.00234

AFIX 43

H17 2 -1.015116 0.771954 0.221217 11.00000 -1.20000

AFIX 0

C10 1 -0.625653 0.972498 0.205938 11.00000 0.02274 0.02073 =
0.01691 -0.00270 0.00203 0.00256

C16 1 -1.278903 0.791617 0.298157 11.00000 0.03839 0.02192 =
0.03113 -0.00244 0.00088 -0.00871

AFIX 43

H16 2 -1.364798 0.741960 0.295766 11.00000 -1.20000

AFIX 0

C12 1 -0.893228 1.019873 0.303575 11.00000 0.02494 0.02102 =
0.01616 -0.00415 0.00005 0.00340

C4 1 0.267800 1.125172 0.002350 11.00000 0.03185 0.02465 =
0.02898 0.00477 0.00721 -0.00599

AFIX 43

H4 2 0.401875 1.140277 -0.029272 11.00000 -1.20000

AFIX 0

C15 1 -1.361158 0.847503 0.347820 11.00000 0.03018 0.03214 =
0.02442 0.00039 0.00476 -0.00087

AFIX 43

H15 2 -1.500034 0.834324 0.378763 11.00000 -1.20000

AFIX 0

O2 5 0.265066 0.873901 0.009398 11.00000 0.02540 0.01870 =
0.03209 -0.00310 0.00671 0.00035

C19 1 -0.952743 1.086481 0.354087 11.00000 0.02164 0.02105 =
0.02016 -0.00326 -0.00429 0.00492

```
O4    5   -1.145286    1.080358    0.396831    11.00000    0.03167    0.02585 =
      0.02718   -0.00897    0.00648   -0.00173
O3    5   -0.801095    1.148828    0.352858    11.00000    0.03257    0.02182 =
      0.02846   -0.00667    0.00815   -0.00021
O5    5    0.338528    0.748540    0.127086    11.00000    0.02905    0.03076 =
      0.03119   -0.00772   -0.00535    0.00005
AFIX   7
H5A   2    0.459159    0.713303    0.139262    11.00000   -1.50000
AFIX   0
H5B   2    0.341639    0.790687    0.150817    11.00000    0.09995
HKLF 4

REM  19101309-1 in P212121 #19
REM R1 =  0.0435 for    3026 Fo > 4sig(Fo)  and  0.0643 for all    3741 data
REM    258 parameters refined using      0 restraints

END

WGHT      0.0307      0.0000

REM Highest difference peak  0.331,  deepest hole -0.430,  1-sigma level  0.077
Q1    1  -0.5154  1.1206  0.2591  11.00000  0.05    0.33
Q2    1  -0.2175  0.8786  0.1608  11.00000  0.05    0.29
Q3    1  -0.8426  1.0020  0.1578  11.00000  0.05    0.29
Q4    1  -0.0629  0.8409  0.0025  11.00000  0.05    0.27
Q5    1   0.0137  0.9183  0.0518  11.00000  0.05    0.26
Q6    1  -0.4466  0.8255  0.1185  11.00000  0.05    0.26
Q7    1   0.1948  0.6999  0.0130  11.00000  0.05    0.26
```

Q8 1 0.3207 0.8972 0.0014 11.00000 0.05 0.25

Q9 1 -0.2677 0.8229 0.1395 11.00000 0.05 0.25

Q10 1 -1.4685 0.7062 0.3581 11.00000 0.05 0.25

Q11 1 0.5663 0.8002 0.1599 11.00000 0.05 0.24

Q12 1 -1.1578 0.8039 0.2799 11.00000 0.05 0.24

Q13 1 -0.0198 0.8968 0.1231 11.00000 0.05 0.24

Q14 1 -0.4282 0.8851 0.1609 11.00000 0.05 0.24

Q15 1 -1.0926 1.1839 0.3431 11.00000 0.05 0.24

Q16 1 0.1728 0.6600 0.0824 11.00000 0.05 0.23

Q17 1 -0.2936 0.7839 0.0920 11.00000 0.05 0.23

Q18 1 0.0871 1.0181 0.0454 11.00000 0.05 0.23

Q19 1 -0.3520 0.9201 0.1001 11.00000 0.05 0.23

Q20 1 0.4220 0.7815 0.0796 11.00000 0.05 0.23

REM The information below was added by Olex2.

REM

REM R1 = 0.0435 for 3026 Fo > 4sig(Fo) and 0.0643 for all 11707 data

REM n/a parameters refined using n/a restraints

REM Highest difference peak 0.33, deepest hole -0.43

REM Mean Shift 0, Max Shift 0.000.

REM +++ Tabular Listing of Refinement Information +++

REM R1_all = 0.0643

REM R1_gt = 0.0435

REM wR_ref = 0.0883

REM GOOF = 1.035

REM Shift_max = 0.000

REM Shift_mean = 0

REM Reflections_all = 11707

REM Reflections_gt = 3026

REM Parameters = n/a

REM Hole = -0.43

REM Peak = 0.33

REM Flack = -0.018(17)

;

_olex2_submission_special_instructions 'No special instructions were received'

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: 19101309-1

```
Bond precision:  C-C = 0.0058 A          Wavelength=0.71073

Cell:            a=4.8722(2)     b=16.6989(6)     c=19.3540(6)
                 alpha=90        beta=90          gamma=90
Temperature:     293 K
```

	Calculated	Reported
Volume	1574.65(10)	1574.65(10)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C20 H12 Mn N2 O5	C20 H12 Mn N2 O5
Sum formula	C20 H12 Mn N2 O5	C20 H12 Mn N2 O5
Mr	415.26	415.26
Dx,g cm-3	1.752	1.752
Z	4	4
Mu (mm-1)	0.879	0.879
F000	844.0	844.0
F000'	845.73	
h,k,lmax	6,22,26	6,21,26
Nref	4263[2485]	3741
Tmin,Tmax	0.760,0.831	0.326,1.000
Tmin'	0.748	

```
Correction method= # Reported T Limits: Tmin=0.326 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 1.51/0.88      Theta(max)= 29.162

R(reflections)= 0.0435( 3026)     wR2(reflections)= 0.0883( 3741)

S = 1.035                 Npar= 258
```

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT222_ALERT_3_C NonSolvent Resd 1  H    Uiso(max)/Uiso(min) Range         4.5 Ratio
PLAT415_ALERT_2_C Short Inter D-H..H-X       H5B       ..H8       .        2.09 Ang.
                                          1+x,y,z  =      1_655 Check
```

Alert level G

```
PLAT004_ALERT_5_G Polymeric Structure Found with Maximum Dimension          3 Info
PLAT007_ALERT_5_G Number of Unrefined Donor-H Atoms ..............          1 Report
PLAT012_ALERT_1_G No       _shelx_res_checksum Found in CIF ......      Please Check
PLAT199_ALERT_1_G Reported _cell_measurement_temperature ..... (K)        293 Check
PLAT200_ALERT_1_G Reported  _diffrn_ambient_temperature ..... (K)         293 Check
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .        1.17 Ratio
PLAT794_ALERT_5_G Tentative Bond Valency for Mn1       (II)       .       2.01 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .      Please Do !
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
   8 ALERT level G = General information/check it is not something unexpected

   4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   1 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
   1 ALERT type 4 Improvement, methodology, query or suggestion
   3 ALERT type 5 Informative message, check
```

Validation response form

Please find below a validation response form (VRF) that can be filled in and pasted into your CIF.

```
# start Validation Reply Form
_vrf_PLAT222_19101309-1
;
PROBLEM: NonSolvent Resd 1  H    Uiso(max)/Uiso(min) Range         4.5 Ratio
RESPONSE: ...
;
_vrf_PLAT415_19101309-1
;
PROBLEM: Short Inter D-H..H-X       H5B       ..H8       .        2.09 Ang.
RESPONSE: ...
;
# end Validation Reply Form
```

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 10/08/2020; check.def file version of 06/08/2020

Datablock 19101309-1 - ellipsoid plot