

Electronic Supplementary Data

Tetraaquabis(4-methoxyphenylacetato-O') magnesium(II) dihydrate and catena-poly[[[(diaqua)manganese(II)]-bis(μ_2 -4-methoxyphenylacetato-O,O')]: A monomeric and a two-dimensional coordination polymer based on 4-methoxyphenylacetic acid

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Table S1 - Bond lengths [Å] and angles [°] of p-methoxyphenylacetate ligand in [Mg(H₂O)₆](C₈H₇O₃)₂·2 H₂O (1)

| | | | |
|----------|------------|----------|------------|
| C1-O1 | 1.262(2) | C4-C5 | 1.386(3) |
| C1-O2 | 1.247(2) | C5-C6 | 1.360(3) |
| C1-C2 | 1.516(2) | C6-O3 | 1.371(2) |
| C2-C3 | 1.509(2) | C6-C7 | 1.386(2) |
| C3-C4 | 1.360(3) | C7-C8 | 1.374(3) |
| C3-C8 | 1.371(3) | C9-O3 | 1.420(3) |
| O2-C1-O1 | 123.92(16) | C6-C5-C4 | 119.9(2) |
| O2-C1-C2 | 118.08(15) | C5-C6-C7 | 118.48(19) |
| O1-C1-C2 | 118.00(15) | C5-C6-O3 | 124.79(19) |
| C3-C2-C1 | 112.65(14) | C7-C6-O3 | 116.73(18) |
| C4-C3-C8 | 116.84(18) | C6-C7-C8 | 121.0(2) |
| C4-C3-C2 | 122.24(17) | C3-C8-C7 | 121.4(2) |
| C8-C3-C2 | 120.92(17) | C6-O3-C9 | 117.51(16) |
| C3-C4-C5 | 122.26(19) | | |

Table S2 - Bond lengths [Å] and angles [°] of p-methoxyphenylacetate ligand in [Mn(H₂O)₂](C₉H₉O₃)₂ (2)

| | | | |
|----------|------------|----------|------------|
| C1-O2 | 1.249(2) | C4-C5 | 1.373(3) |
| C1-O1 | 1.260(2) | C5-C6 | 1.380(3) |
| C1-C2 | 1.509(3) | C6-O3 | 1.365(2) |
| C2-C3 | 1.504(3) | C6-C7 | 1.381(3) |
| C3-C8 | 1.380(3) | C7-C8 | 1.383(3) |
| C3-C4 | 1.383(3) | C9-O3 | 1.419(3) |
| O2-C1-O1 | 122.77(17) | C4-C5-C6 | 120.43(19) |
| O2-C1-C2 | 119.08(16) | O3-C6-C5 | 115.53(18) |
| O1-C1-C2 | 118.13(15) | O3-C6-C7 | 125.32(19) |
| C3-C2-C1 | 115.60(16) | C5-C6-C7 | 119.15(18) |
| C8-C3-C4 | 117.28(17) | C6-C7-C8 | 119.53(19) |
| C8-C3-C2 | 121.64(19) | O3-C8-C7 | 122.02(19) |
| C4-C3-C2 | 121.04(19) | C6-O3-C9 | 117.78(17) |
| C5-C4-C3 | 121.57(19) | | |

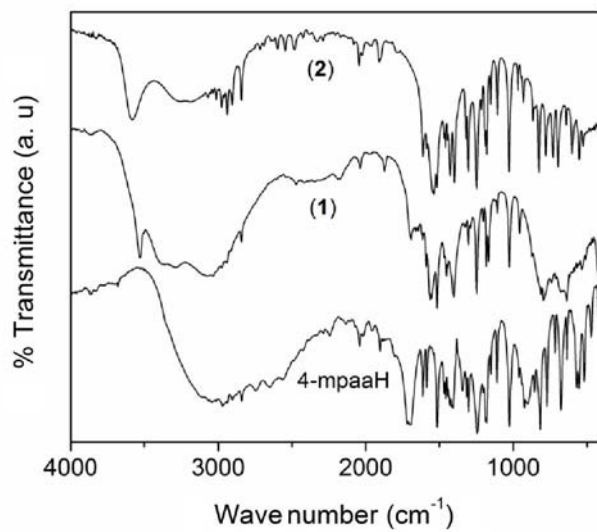


Fig. S1- The IR spectra of mpaH (bottom), $[\text{Mg}(\text{H}_2\text{O})_4(\text{C}_9\text{H}_9\text{O}_3)_2] \cdot 2\text{H}_2\text{O}$ (1) and $[\text{Mn}(\text{H}_2\text{O})_2(\text{C}_9\text{H}_9\text{O}_3)_2]$ (2).

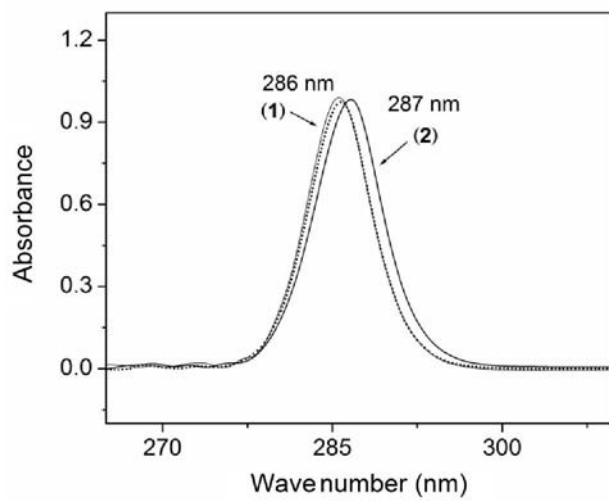


Fig. S2 - The UV-Visible spectra of p-mpaH (dotted line), $[\text{Mg}(\text{H}_2\text{O})_4(\text{C}_9\text{H}_9\text{O}_3)_2] \cdot 2\text{H}_2\text{O}$ (1) and $[\text{Mn}(\text{H}_2\text{O})_2(\text{C}_9\text{H}_9\text{O}_3)_2]$ (2).

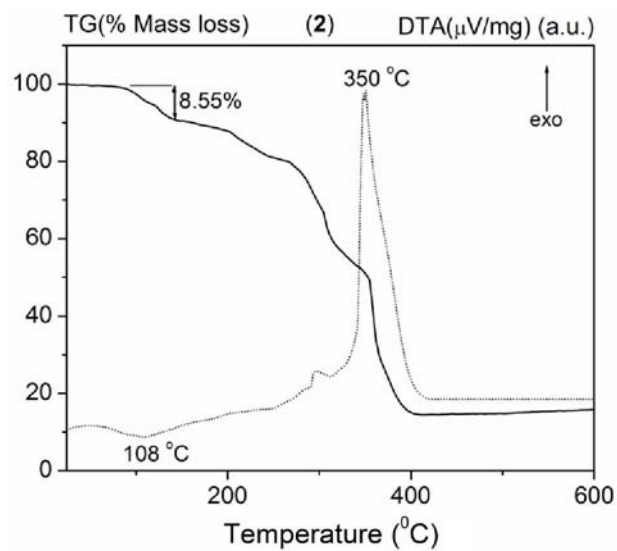


Fig. S3 - The TG-DTA of $[\text{Mn}(\text{H}_2\text{O})_2(\text{C}_9\text{H}_9\text{O}_3)_2]$ (**2**).

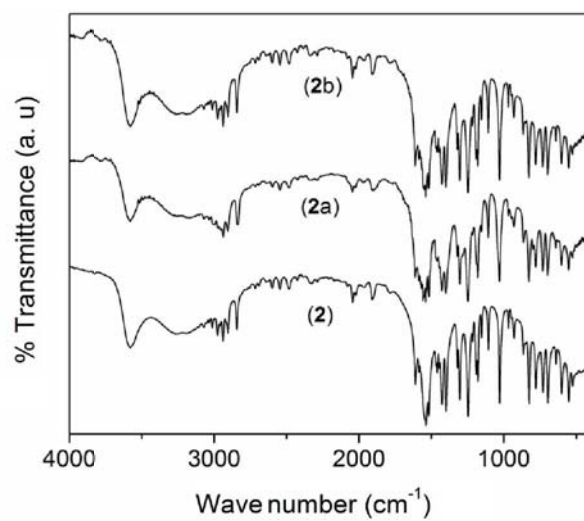


Fig. S4 - The Infrared spectra of compounds (**2**), **2a** (heated above 120 °C), **2b** (rehydrated) showing reversible hydration.

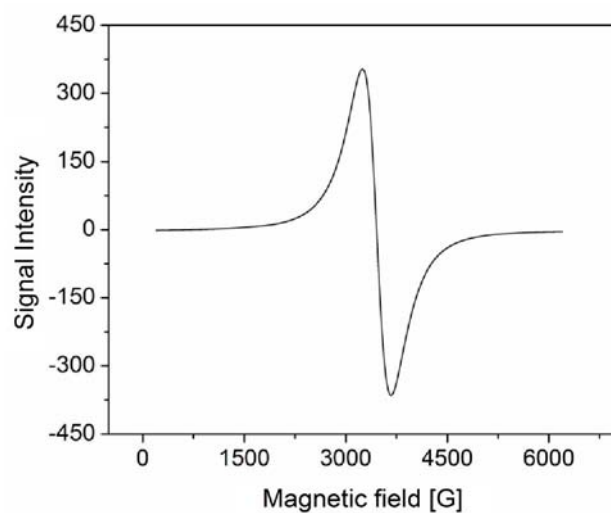


Fig. S5 - ESR spectra of $[\text{Mn}(\text{H}_2\text{O})_2(\text{C}_9\text{H}_9\text{O}_3)_2]$ (**2**)

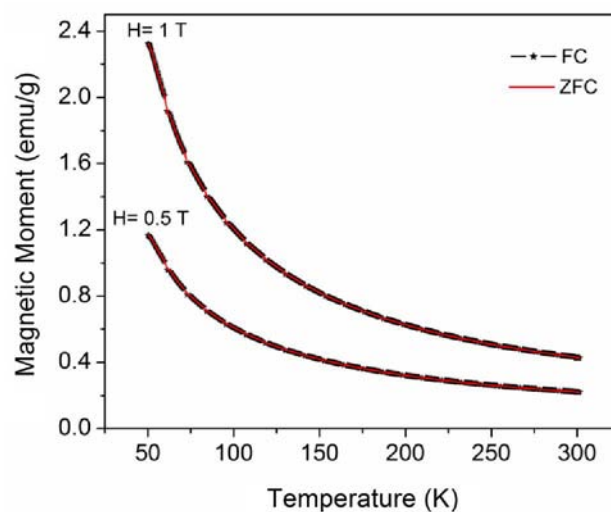


Fig. S6 - Magnetization vs Temperature (M-T) curve of $[\text{Mn}(\text{H}_2\text{O})_2(\text{C}_9\text{H}_9\text{O}_3)_2]$ (**2**)

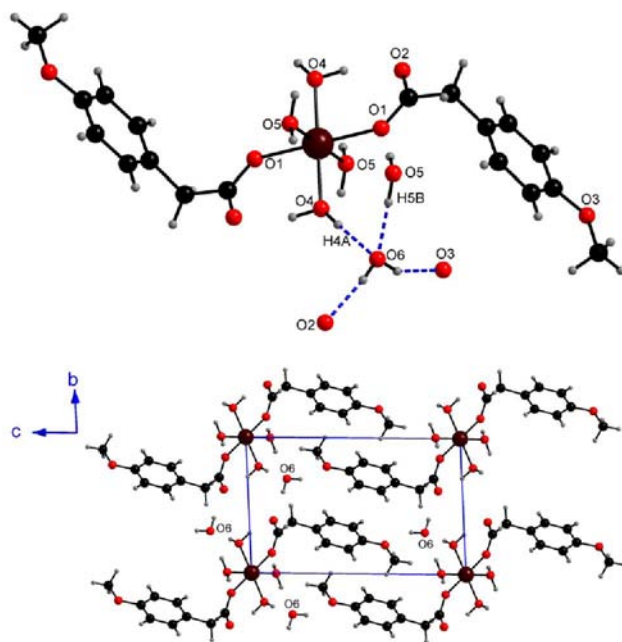


Fig. S7 - A view (**top**) of the H-bonding surroundings of the lattice water showing the linking of four different Mg(II) complexes with the aid of O-H \cdots O interactions. For symmetry relations see Table 3. The crystallographic packing of the unit cell of $[\text{Mg}(\text{H}_2\text{O})_4(\text{C}_6\text{H}_9\text{O}_3)_2] \cdot 2\text{H}_2\text{O}$ (**1**) viewed along a axis. O6 is the lattice water. (**bottom**)

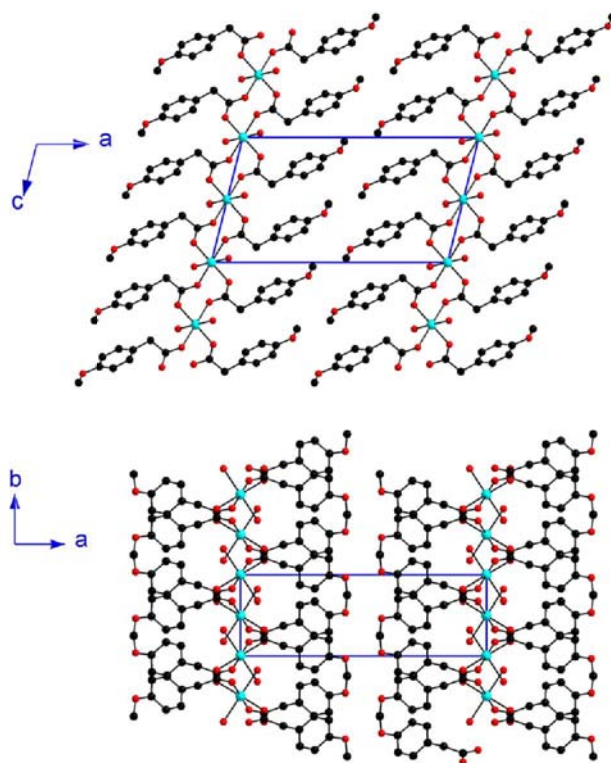


Fig. S8 - A view along b axis showing the extended chain of the Mn(II) ions along c axis due to the μ_2 -bridging bidentate mode of the 4-mpa ligand. Note that along a there is a break (**top**). A view along c axis showing the extended chain of the Mn(II) ions along b axis due to the μ_2 -bridging bidentate. Note that along a there is a break (**bottom**)

checkCIF/PLATON report for [Mg(H₂O)₄(C₉H₉O₃)₂].2H₂O (1)

Structure factors have been supplied for datablock(s) 1

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: 1

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=5.3462(3) b=8.2219(4) c=12.8416(7)
alpha=85.249(2) beta=81.336(2) gamma=77.271(2)

Temperature: 293 K

| | Calculated | Reported |
|------------------------|-------------------------|-------------------------|
| Volume | 543.59(5) | 543.59(5) |
| Space group | P -1 | P -1 |
| Hall group | -P 1 | -P 1 |
| Moiety formula | C18 H26 Mg O10, 2(H2 O) | C18 H26 Mg O10, 2(H2 O) |
| Sum formula | C18 H30 Mg O12 | C18 H30 Mg O12 |
| Mr | 462.73 | 462.73 |
| Dx, g cm ⁻³ | 1.413 | 1.414 |
| Z | 1 | 1 |
| Mu (mm ⁻¹) | 0.144 | 0.144 |
| F000 | 246.0 | 246.0 |
| F000' | 246.20 | |
| h, k, lmax | 6, 10, 15 | 6, 10, 15 |
| Nref | 2137 | 2131 |
| Tmin, Tmax | 0.951, 0.958 | 0.696, 0.746 |
| Tmin' | 0.951 | |

Correction method= MULTI-SCAN

Data completeness= 0.997 Theta(max)= 25.995

R(reflections)= 0.0414(1850) wR2(reflections)= 0.1167(2131)

S = 1.065 Npar= 167

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

| | | | |
|-------------------|---|--|-----------|
| PLAT241_ALERT_2_C | High | Ueq as Compared to Neighbors for | C7 Check |
| PLAT242_ALERT_2_C | Low | Ueq as Compared to Neighbors for | C3 Check |
| PLAT242_ALERT_2_C | Low | Ueq as Compared to Neighbors for | C6 Check |
| PLAT250_ALERT_2_C | Large U3/U1 Ratio for Average U(i,j) Tensor | | 2.2 Note |
| PLAT334_ALERT_2_C | Small Average Benzene C-C Dist. C3 | -C8 | 1.37 Ang. |
| PLAT911_ALERT_3_C | Missing # FCF Refl Between THmin & STh/L= | 0.600 | 6 Report |

Alert level G

| | | | |
|-------------------|--|------|----------------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | | 9 Note |
| PLAT154_ALERT_1_G | The su's on the Cell Angles are Equal | | 0.00200 Degree |
| PLAT172_ALERT_4_G | The CIF-Embedded .res File Contains DFIX Records | | 2 Report |
| PLAT199_ALERT_1_G | Reported cell measurement temperature | (K) | 293 Check |
| PLAT200_ALERT_1_G | Reported _diffrn_ambient_temperature | (K) | 293 Check |
| PLAT790_ALERT_4_G | Centre of Gravity not Within Unit Cell: Resd. # | H2 O | 2 Note |
| PLAT860_ALERT_3_G | Number of Least-Squares Restraints | | 9 Note |
| PLAT910_ALERT_3_G | Missing # of FCF Reflections Below Th(Min) | | 1 Report |

0 **ALERT level A** = Most likely a serious problem - resolve or explain 0

ALERT level B = A potentially serious problem, consider carefully

6 **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

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data

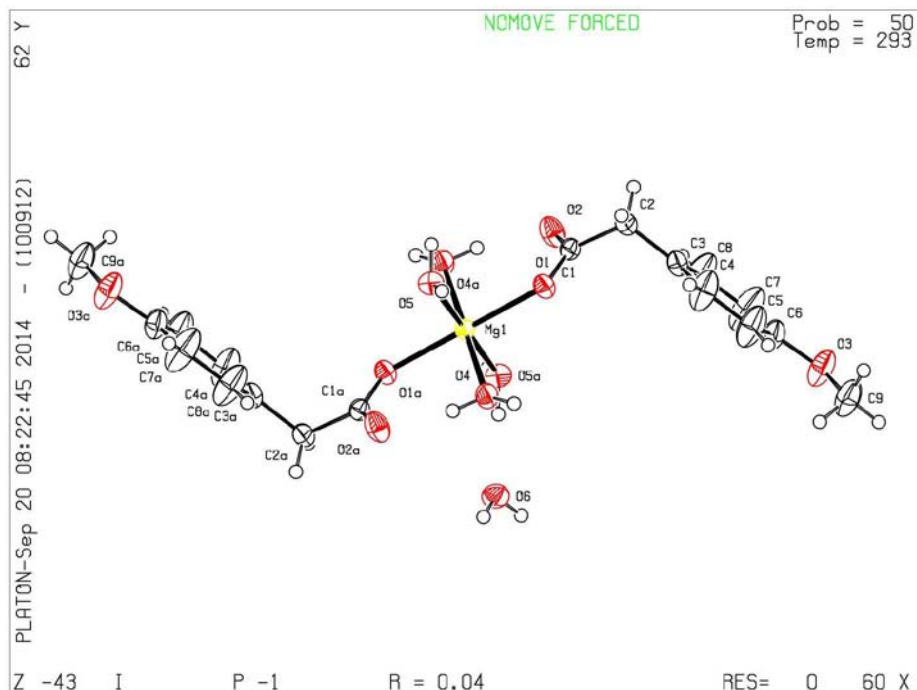
6 ALERT type 2 Indicator that the structure model may be wrong or deficient

3 ALERT type 3 Indicator that the structure quality may be low

2 ALERT type 4 Improvement, methodology, query or suggestion

0 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014



checkCIF/PLATON report for [Mn(H₂O)₂(C₉H₉O₃)₂] (2)

Structure factors have been supplied for datablock(s) (2)

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: (2)

Bond precision: C-C = 0.0030 A Wavelength=0.71073

Cell: a=17.5084 (7) b=5.6246 (3) c=9.2334 (2)
 alpha=90 beta=104.711 (3) gamma=90

Temperature: 293 K

| | Calculated | Reported |
|------------------------|---------------|---------------|
| Volume | 879.48 (6) | 879.48 (6) |
| Space group | P 21/c | P 21/c |
| Hall group | -P 2ybc | -P 2ybc |
| Moiety formula | C18 H22 Mn O8 | C18 H22 Mn O8 |
| Sum formula | C18 H22 Mn O8 | C18 H22 Mn O8 |
| Mr | 421.30 | 421.29 |
| Dx, g cm ⁻³ | 1.591 | 1.591 |
| Z | 2 | 2 |
| Mu (mm ⁻¹) | 0.796 | 0.796 |
| F000 | 438.0 | 438.0 |
| F000' | 438.91 | |
| h, k, lmax | 21, 6, 11 | 21, 6, 11 |
| Nref | 1716 | 1716 |
| Tmin, Tmax | 0.788, 0.820 | 0.796, 0.826 |
| Tmin' | 0.788 | |

Correction method= MULTI-SCAN

Data completeness= 1.000 Theta (max)= 25.996

R(reflections)= 0.0278 (1393) wR2(reflections)= 0.0714 (1716)

S = 1.046 Npar= 133

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

PLAT480_ALERT_4_C Long H...A H-Bond Reported H9B .. O3 .. 2.63 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H9B .. O3 .. 2.63 Ang.
PLAT790_ALERT_4_C Centre of Gravity not Within Unit Cell: Resd. # 1 Note
C18 H22 Mn O8
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.938 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 3 Note
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension 2 Info
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 2 Report
PLAT199_ALERT_1_G Reported _cell_measurement_temperature (K) 293 Check
PLAT200_ALERT_1_G Reported diffn ambient temperature (K) 293 Check
PLAT860_ALERT_3_G Number of Least-Squares Restraints 3 Note
PLAT910_ALERT_3_G Missing # of FCF Reflections Below Th(Min) 1 Report

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ALERT level B = A potentially serious problem, consider carefully
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ALERT level G = General information/check it is not something unexpected

2 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
3 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

PLATON version of 20/08/2014; check.def file version of 18/08/2014

Datablock I - ellipsoid plot

