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Synthesis, Crystal Structure and Photoluminescence Properties of Diaquabis (1,10Phenanthroline, κ,N,N')(Benzoato-κ,O) Manganese(II)Dihydrate

Idongesit Justina Mbonu[1,2]*, Olusegun Kehinde Abiola[1], Kenneth Abara Ibe[1], Doris Fovwe Ogeleka[1] and Elias E Elemike[1]

[1]*Department of Chemistry, Federal University of Petroleum Resources, Nigeria*

[2]*Department of Chemistry, University of Utah, United States*

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***Corresponding author:** Idongesit Justina Mbonu, Department of Chemistry, Federal University of Petroleum Resources, P.M.B.1221 Effurun, Delta State Nigeria

Abstract

A new complex, $Mn_3(C_7H_4O_2)_2(C_{12}H_8N_2)(CH_3OH)_2(H_2O)_4$, has been synthesized under slow solvent evaporation method. The compound was characterized by photoluminescence and single crystal X-ray diffraction techniques. The compound gives triclinic structure with a space group P-1(No. 2). The observed unit cell dimensions are a = 7.4369(3)Å, b= 12.9898(6)Å, c = 14.1176(6)Å, α =88.847(2)°, β =82.518(2)°, γ = 89.975(2)° , V = 1351.93(10)Å^3, and Z = 2. Its asymmetric unit consists of centrosymmetric trinuclear MnII cation, four water molecules, four oxygen atoms from benzoate dianion and 1, 10- phenanthroline molecule. Each of the MnII cations is six-coordinated forming octahedral geometry. The crystal packing of the prepared compound is stabilized by strong intermolecular hydrogen bonds forming 2D structure which further engaged in a weak C —H...O, C—N---O, O—H...O and N—H....O hydrogen bonding to create a 3D network. The determined molar conductance in DMSO solution was 9.35Ω^{-1}cm^{2}mol^{-1} indicating a non-electrolyte behavior of this compound. Mn-MOF shows fluorescence in solution ranging from 324-460nm revealing its efficient room-temperature phosphorescence in chloroform with a remarkable weak quenching by molecular oxygen, an indication that this compound can be used in fields such as drugs industries, energy storage systems, as luminescence sensors to analyze water, air and chemical pollutions.

Keywords: Crystal structure; 1, 10-phenanthroline; Benzoate anion; Mn^{II} complex; Photoluminescence

Introduction

Colossal works have been done towards the design and preparation of coordination polymers that are porous because of their captivating structures and their imminent applications in luminescence, electronics, catalysis, energy storage, sensors, and partitioning [1,2]. Metal-carboxylates and metal-o-phenanthroline with their derivatives are outstanding due to their interesting highlights and properties [3,4]. Our past work sums up detailed synthesis, structural impact variables, and properties of Mn-MOF. Over the last two decades coordination chemists have been devoted to the study of artificial systems by trying to mimic the natural photosynthesis processes. All aspirations has been on how to exploit electronic states of metal complexes and develop them into supramolecular systems with various electron acceptors and donors for applications in photo catalysis, sensoring, luminescence probes, biomedical applications ,and energy storage in order to reduce pollution in our society, In situations whereby the fluorescence emission red-shift with regards to the wavelength of excitation source, information from the signal gives the intensity, wavelength, lifetime and polarization as in regards to the environment of the fluorophore.

Organic compounds are limited in their use because they are thermally unstable and limited in their capacity in terms of electron transfer and transport processes [5,6]. Inorganic compounds even when they are thermally stable cannot be easily processed because of this they are limited in their versatility When inorganic and organic compounds are combined together, new framework with improved and enhanced properties are formed towards high capacity participation in "electron transfer and transport" leading to versatility in applications. In continuation of our past work, we report new manganese coordination metal-organic framework

$[Mn_3(C_7H_4O_2)_2(C_{12}H_8N_2)\ (CH_3OH)_2(H_2O)_4]$, resulting from the reaction of benzoic acid and Mn^{II} ions with 1,10- phenanthroline. The asymmetric unit of Mn-MoF consists of centrosymmetric trinuclear Mn^{II} cation, four water molecules, four oxygen atoms from benzoate dianion and 1,10 phenanthroline molecule (Figure1).

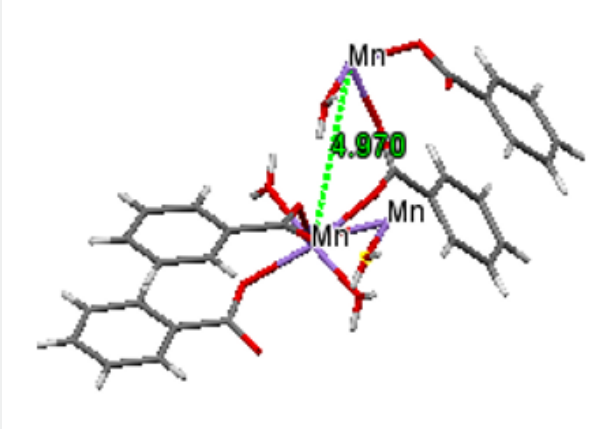

Figure 1: Asymmetric unit of Mn-MOF.

Materials and Methods

The different coordination modes of the manganese transition metal with 1,10 phenanthroline and carboxylic acids was determined [7,8,9]. Bond distance, bond angle values were determined [9]. The identification of chiral center(s) and their (R/S)-configuration were also carried out [10]. Selected bond lengths (Å) were used for elucidating the structure of Mn-MOF [11,12].

The following crystallographic tools were used to calculate and determine the geometrical properties of the crystal structure of Mn-MOF. The cell dimensions, space group symmetry, structure refinement and data reduction for Mn-MOF were computed by APEX2, SAINT, SHELXL-2018/3, respectively. The molecular graphics was prepared using SHELXL and PLATON (V-260918) software [13,14]. The Mn-MOF atom refinement was done by invariom refinement and molecular electron-density distribution constructed from 'Hansen/Coppens' multipole-mode parameter values as given in Table 1. The electron density of the asymmetric unit is obtained by a single-point energy calculation.

Table 1: Crystal data, data collection and structure refinement of Mn-MOF at 200 K.

Crystal Data	
Empirical formula	$C_{28}H_{32}Mn_3O_{12}N_2$
Formula weight	753.37
Unit Cell Weight	1332.77
Crystal system	triclinic
Space group	P-1(No.2)
a/Å, α/°	7.4369(3), 88.847(2)
b/Å, β/°	12.9898(6), 82.518(2)
c/Å, γ/°	14.1176(6), 89.975(2)
Volume/Å^3	1351.93(10)
Z	2
ρ calc/g cm^{-3}	1.637
μ/mm^{-1}	1.001
F (000)	684 [calc. 685.70]
Crystal size/mm^3	0.05 x 0.54 x 0.60
Data Collection	

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Temperature/K	200
Theta Min-Max/°	1.6, 28.4
Dataset /restraints/parameters	-9: 9; -16: 17; -18: 18
Tot., Uniq. Data, R(int)	49223, 6713, 0.025
Observed Data [I ≥ 2.0σ (I)]	5021
Refinement	
Nref, Npar	6713, 414
R, wR2, S	0.0353, 0.1092, 1.05
w = ^2^(FO^2^) +(0.0551P) ^2^+1.0319P] Where P=(FO^2^+2FC^2^)/3'	
Max. and Av. Shift/Error	0.00, 0.00
Min. and Max. Resd. Dens. [e/Ang^3]	-0.56, 1.34
Radiation/ Å MoKα	0.71073

Preparation of Mn-MOF

The mixture of $MnCl_2.4H_2O$ (0.5 mmol) and benzoic acid (0.1 mmol) in 10 mL aqueous solution was stirred for about [15] 5 minutes to give a red solution at 50 °C. The mixture was kept at a pH 7 by the slow addition of a NaOH solution (1mol/L). A 5 mL methanol solution of 1, 10-phenanthroline (0.5 mmol) was added and the solution was stirred and heated for 3h at 50 °C, followed by filtration. The pale-yellow crystals were separated by slow evaporation at room temperature after 5 days [16]. The results of elemental analyses show that the C, H, Mn, and O are 50.50, 4.20, 16.50, and 28.80 (calc.) and 50.48, 4.27, 16.40, and 28.85 (found), respectively.

Single-crystal X-ray diffraction

Plate-like yellow single-crystals of Mn-MOF of 0.05 x 0.54 x 0.60 mm^3 crystal size dimensions (Table 1) were chosen for X-ray diffraction measurement. Cell dimensions, space group symmetry, structure refinement (SAINT program: Bruker, 2009) and data reduction for Mn-MOF were computed using SHELXL-2018/3 software program [17] and results summarized in Tables 1-11. The structure of Mn-MOF was solved via SIR92 program application to be triclinic, P-1(No.2) space group and calculated density of 1.637g/cm^3 primarily based on five molecules packed in the unit-cell volume of 1351.93(10) $Å^3$ and this information used to evaluate the position of each elements in the molecule.

Final Coordinates and Equivalent Isotropic Displacement Parameters were used for the non-Hydrogen atoms (Table 2). The hydrogen atoms coordinated to benzene rings (C—H = 0.9500Å) in Mn-MOF (Table 3) have been fixed in a geometrical order. The refinement on the crystal structure of Mn-MOF was achieved by applying the' riding model' with isotropic displacements (Tables 2,4,5). All information on the geometric parameters used in characterizing the molecular structure of Mn-MOF is found in supporting information, Tables 2-11. SHELXL [17] and PLATON (V-260918) have been used to prepare the molecular graphics of the compound for publication. The construction of Mn-MOF structures is proven in Figures 1-3.

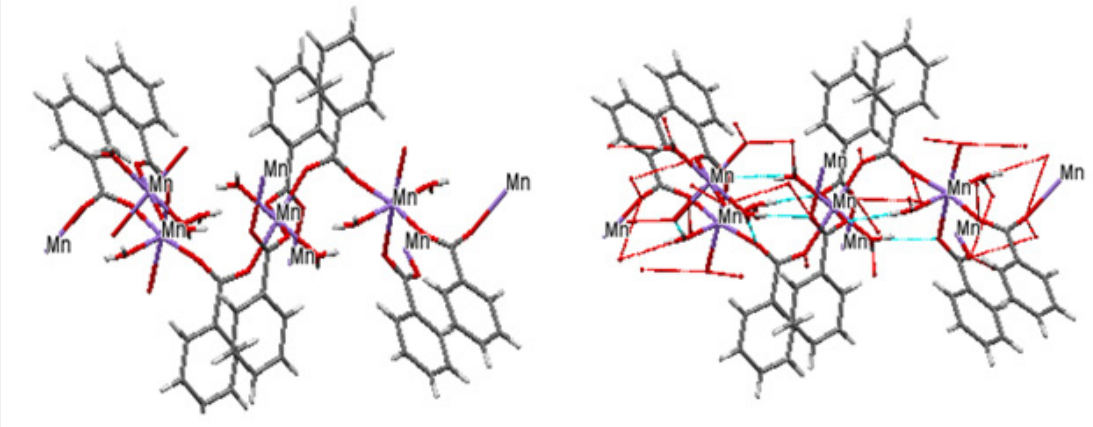

Figure 2: Molecular structure and 50% displacement ellipsoids of Mn-MOF.

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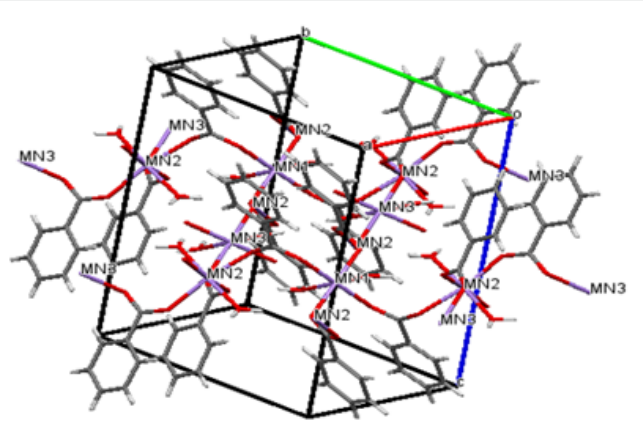

Figure 3: Crystal packing of Mn-MOF showing 3D network: H atoms intermolecular interaction omitted for clarity.

Table 2: Final Coordinates and Equivalent Isotropic Displacement Parameters of the non-Hydrogen atoms.

Atom	X	Y	Z	U(eq)Å²
Mn2	0.50581(3)	0.25000(2)	0.49981(2)	0.0144(1)
Mn3	0	1/2	1/2	0.0146(1)
O5	-0.00591(18)	0.14659(11)	0.57271(11)	0.0242(4)
O6	0.51326(18)	0.40025(11)	0.42696(11)	0.0240(4)
O7	0.47709(18)	0.09973(11)	0.57230(11)	0.0240(4)
O8	-0.03022(18)	0.64659(11)	0.57254(11)	0.0244(4)
O11	-0.20628(17)	0.05453(11)	0.41481(10)	0.0217(4)
O12	-0.25926(17)	0.22119(11)	0.39367(10)	0.0217(4)
O21	0.22954(17)	0.03774(11)	0.39453(10)	0.0215(4)
O22	0.30622(17)	0.20135(11)	0.41002(10)	0.0225(4)
O31	0.68769(17)	0.27869(11)	0.60571(10)	0.0219(4)
O32	0.75086(17)	0.44525(10)	0.58434(10)	0.0213(4)
O41	0.26212(17)	0.29875(11)	0.59028(10)	0.0225(4)
O42	0.17674(18)	0.46219(10)	0.60601(10)	0.0216(4)
C11	-0.0922(2)	0.13198(15)	0.26549(14)	0.0195(5)
C12	-0.0535(3)	0.03716(17)	0.0274(6)	0.0274(6)
C13	0.0365(3)	0.0326(2)	0.13148(18)	0.0385(8)
C14	0.0915(3)	0.1217(2)	0.08147(17)	0.0372(8)
C15	0.0565(3)	0.2158(2)	0.12284(17)	0.0346(7)
C16	-0.0372(3)	0.22182(17)	0.21423(15)	0.0264(6)
C17	-0.1928(2)	0.13639(14)	0.36461(13)	0.0160(5)
C21	0.4089(2)	0.12004(15)	0.26416(14)	0.0195(5)
C22	0.4412(3)	0.02850(17)	0.21575(15)	0.0269(6)
C23	0.5348(3)	0.0296(2)	0.12409(18)	0.0388(8)
C24	0.5940(3)	0.1210(2)	0.08033(17)	0.0400(8)
C25	0.5631(3)	0.2121(2)	0.12776(18)	0.0383(8)
C26	0.4712(3)	0.21230(17)	0.21999(16)	0.0273(6)
C27	0.3075(2)	0.11996(14)	0.36317(13)	0.0160(5)

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C31	0.7903(2)	0.36826(15)	0.73382(14)	0.0191(5)
C32	0.8075(3)	0.46326(17)	0.77502(16)	0.0272(6)
C33	0.8523(3)	0.4684(2)	0.86716(18)	0.0377(8)
C34	0.8838(3)	0.3793(2)	0.91732(16)	0.0367(8)
C35	0.8699(3)	0.2852(2)	0.87641(16)	0.0339(7)
C36	0.8210(3)	0.27872(17)	0.78500(15)	0.0261(6)
C37	0.7392(2)	0.36375(14)	0.63466(13)	0.0155(5)
C41	0.2913(2)	0.37981(15)	0.73649(14)	0.0194(5)
C42	0.2985(3)	0.47099(17)	0.78517(15)	0.0271(6)
C43	0.3460(3)	0.4698(2)	0.87698(17)	0.0384(8)
C44	0.3830(3)	0.3779(2)	0.92070(17)	0.0414(8)
C45	0.3762(3)	0.2872(2)	0.87296(17)	0.0381(8)
C46	0.3315(3)	0.28741(18)	0.78020(16)	0.0276(6)
C47	0.2396(2)	0.38016(14)	0.63722(13)	0.0161(5)

U(eq) = 1/3 of trace orthogonalized U Tensor.

Table 3: Bond Distances (Á).

Mn1-O5	2.1791(15)	O6	-H6A	0.841(18)
Mn1-O11	2.1787(13)	O6	-H6B	0.841(18)
Mn1-O21	2.1635(13)	O7	-H7B	0.839(18)
Mn1-O5_c	2.1791(15)	O7	-H7A	0.843(18)
Mn1- O11_c	2.1787(13)	O8	-H8A	0.843(18)
Mn1-O21_c	2.1635(13)	O8	-H8B	0.843(19)
Mn2-O6	2.1851(15)	C11	-C17	1.501(3)
Mn2-O7	2.1832(15)	C11	-C12	1.387(3)
Mn2-O22	2.1754(14)	C11	-C16	1.394(3)
Mn2-O31	2.1802(14)	C12	-C13	1.393(3)
Mn2-O41	2.1784(14)	C13	-C14	1.378(4)
Mn2-O12_b	2.1859(14)	C14	-C15	1.375(4)
Mn3-O8	2.1779(15)	C15	-C16	1.388(3)
Mn3-O42	2.1658(14)	C21	-C26	1.391(3)
Mn3-O32_a	2.1792(13)	C21	-C27	1.499(3)
Mn3-O8_d	2.1779(15)	C21	-C22	1.389(3)
Mn3-O42_d	2.1658(14)	C22	-C23	1.387(3)
Mn3-O32_e	2.1792(13)	C23	-C24	1.373(4)
O11-C17	1.263(2)	C24	-C25	1.376(4)
O12-C17	1.261(2)	C25	-C26	1.390(3)
O21-C27	1.260(2)	C31	-C32	1.388(3)
O22-C27	1.258(2)	C31	-C36	1.391(3)
O31-C37	1.263(2)	C31	-C37	1.500(3)
O32-C37	1.260(2)	C32	-C33	1.387(3)
O41-C47	1.259(2)	C33	-C34	1.381(4)
O42-C47	1.258(2)	C34	-C35	1.372(4)
O5-H5B	0.840(19)	C35	-C36	1.390(3)
O5-H5A	0.84(2)	C41	-C46	1.389(3)

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C41-C47	1.501(3)	C24	-H24	0.95
C41-C42	1.386(3)	C25	-H25	0.95
C42-C43	1.387(3)	C26	-H26	0.95
C43-C44	1.377(4)	C32	-H32	0.95
C44-C45	1.373(4)	C33	-H33	0.95
C45-C46	1.392(3)	C34	-H34	0.95
C12-H12	0.95	C35	-H35	0.95
C13-H13	0.95	C36	-H36	0.95
C14-H14	0.95	C42	-H42	0.95
C15-H15	0.95	C43	-H43	0.95
C16-H16	0.95	C44	-H44	0.95
C22-H22	0.95	C45	-H45	0.95
C23-H23	0.95	C46	-H46	0.95

Table 4: Hydrogen Atom Positions and Isotropic Displacement Parameters.

Atom	X	Y	Z	Uiso Å²
H5A	-0.099(2)	0.1837(19)	0.582(2)	0.062(10)
H5B	0.081(2)	0.1882(17)	0.571(2)	0.048(8)
H6A	0.609(2)	0.4349(17)	0.426(2)	0.043(8)
H6B	0.431(2)	0.4442(16)	0.424(2)	0.042(8)
H7A	0.572(2)	0.0655(19)	0.577(2)	0.055(9)
H7B	0.393(2)	0.0563(16)	0.575(2)	0.044(8)
H8A	-0.115(2)	0.6898(16)	0.573(2)	0.046(8)
H8B	0.060(2)	0.6813(19)	0.584(2)	0.054(9)
H12	-0.08824	-0.02453	0.25905	0.033
H13	0.06013	-0.03224	0.10258	0.046
H14	0.15351	0.11814	0.0184	0.045
H15	0.0967	0.27701	0.08864	0.042
H16	-0.06374	0.28709	0.24181	0.032
H22	0.39917	-0.03486	0.24541	0.032
H23	0.55802	-0.03321	0.09142	0.047
H24	0.65643	0.12132	0.01717	0.048
H25	0.60484	0.27518	0.09734	0.046
H26	0.45093	0.27525	0.25278	0.033
H32	0.78863	0.52475	0.74013	0.033
H33	0.86137	0.53342	0.89582	0.045
H34	0.91518	0.3832	0.98027	0.044
H35	0.89375	0.22411	0.91077	0.041
H36	0.80866	0.21336	0.75752	0.031
H42	0.27085	0.53438	0.75564	0.033
H43	0.35303	0.53248	0.90978	0.046
H44	0.41321	0.37726	0.98404	0.05
H45	0.40214	0.22404	0.90337	0.046
H46	0.3285	0.22467	0.74699	0.033

The Temperature Factor has the Form of Exp(-T).
Where, T = 8*(Pi**2)*U*(Sin(θ)/λ)**2 for Isotropic Atoms.

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Table 5: Isotropic Displacement Parameters (Á²).

Atom	U (1,1) or U	U (2,2)	U (3,3)	U (2,3)	U (1,3)	U (1,2)
Mn1	0.0122(2)	0.0134(2)	0.0176(2)	0.0002(1)	-0.0006(1)	0.0001(13)
Mn2	0.0124(1)	0.0129(2)	0.0180(2)	-0.0015(1)	-0.0019(1)	-0.0001(10)
Mn3	0.0133(2)	0.0132(2)	0.0175(2)	0.0003(1)	-0.0029(1)	-0.0008(13)
O5	0.0161(6)	0.0176(7)	0.0386(9)	-0.0066(6)	-0.0018(6)	-0.0010(5)
O6	0.0167(6)	0.0167(7)	0.0386(9)	0.0032(6)	-0.0042(6)	-0.0009(5)
O7	0.0157(6)	0.0177(7)	0.0391(9)	0.0032(6)	-0.0058(6)	-0.0009(5)
O8	0.0176(6)	0.0177(7)	0.0392(9)	-0.0069(6)	-0.0079(6)	0.0023(5)
O11	0.0168(6)	0.0218(7)	0.0266(7)	0.0046(6)	-0.0041(5)	-0.0011(5)
O12	0.0169(6)	0.0205(7)	0.0271(8)	-0.0062(6)	0.0006(5)	0.0012(5)
O21	0.0180(6)	0.0199(7)	0.0250(7)	0.0019(6)	0.0027(5)	-0.0021(5)
O22	0.0176(6)	0.0229(7)	0.0281(8)	-0.0095(6)	-0.0054(5)	0.0008(5)
O31	0.0195(6)	0.0204(7)	0.0271(8)	-0.0064(6)	-0.0071(5)	0.0004(5)
O32	0.0167(6)	0.0204(7)	0.0265(7)	0.0043(6)	-0.0024(5)	-0.0004(5)
O41	0.0178(6)	0.0226(7)	0.0270(7)	-0.0097(6)	-0.0008(5)	0.0013(5)
O42	0.0219(6)	0.0190(7)	0.0250(7)	0.0024(5)	-0.0082(5)	0.0005(5)
C11	0.0141(8)	0.0240(10)	0.0208(9)	-0.0022(7)	-0.0037(7)	0.0028(7)
C12	0.0269(10)	0.0281(11)	0.0272(11)	-0.0052(9)	-0.0029(8)	0.0036(8)
C13	0.0353(12)	0.0471(15)	0.0333(13)	0.0172(11)	0.0030(10)	0.0111(10)
C14	0.0242(10)	0.0660(18)	0.0203(11)	0.0047(11)	0.0017(8)	0.0049(10)
C15	0.0289(11)	0.0475(15)	0.0268(12)	0.0112(10)	-0.0028(9)	-0.0039(9)
C16	0.0236(9)	0.0290(11)	0.0263(11)	0.0022(8)	-0.0021(8)	0.0002(8)
C17	0.0109(7)	0.0180(9)	0.0197(9)	-0.0009(7)	-0.0047(6)	0.0005(6)
C21	0.0129(7)	0.0247(10)	0.0213(9)	-0.0006(7)	-0.0037(7)	-0.0013(7)
C22	0.0246(9)	0.0297(11)	0.0259(11)	-0.0041(9)	-0.0013(8)	0.0000(8)
C23	0.0333(12)	0.0526(16)	0.0296(12)	0.0147(11)	0.0009(9)	0.0034(11)
C24	0.0246(10)	0.074(2)	0.0196(11)	0.0032(11)	0.0028(8)	-0.0039(11)
C25	0.0284(11)	0.0541(16)	0.0318(13)	0.0193(11)	-0.0047(9)	-0.0125(10)
C26	0.0236(9)	0.0296(11)	0.0287(11)	0.0051(9)	-0.0047(8)	-0.0047(8)
C27	0.0104(7)	0.0186(9)	0.0197(9)	-0.0011(7)	-0.0047(6)	0.0004(6)
C31	0.0129(7)	0.0242(10)	0.0199(9)	-0.0018(7)	-0.0011(6)	-0.0025(6)
C32	0.0271(10)	0.0273(11)	0.0275(11)	-0.0059(9)	-0.0038(8)	-0.0031(8)
C33	0.0373(12)	0.0442(15)	0.0326(13)	0.0157(11)	0.0064(10)	-0.0047(10)
C34	0.0269(10)	0.0646(17)	0.0194(11)	0.0050(11)	-0.0059(8)	-0.0022(10)
C35	0.0276(10)	0.0465(14)	0.0272(12)	0.0118(10)	-0.0046(9)	0.0000(9)
C36	0.0244(9)	0.0282(11)	0.0259(11)	0.0015(8)	-0.0045(8)	-0.0010(8)
C37	0.0083(7)	0.0186(9)	0.0190(9)	-0.0009(7)	0.0008(6)	-0.0012(6)
C41	0.0121(7)	0.0256(10)	0.0200(9)	-0.0014(7)	-0.0005(6)	0.0011(7)
C42	0.0260(10)	0.0297(11)	0.0262(11)	-0.0043(9)	-0.0051(8)	-0.0007(8)
C43	0.0348(12)	0.0533(16)	0.0285(12)	0.0150(11)	-0.0070(9)	-0.0033(11)
C44	0.0267(11)	0.077(2)	0.0214(11)	0.0034(12)	-0.0071(9)	-0.0002(11)
C45	0.0281(11)	0.0549(16)	0.0307(12)	0.0195(11)	-0.0046(9)	0.0047(10)
C46	0.0235(9)	0.0307(11)	0.0281(11)	0.0052(9)	-0.0022(8)	0.0031(8)

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C47	0.0099(7)	0.0183(9)	0.0195(9)	-0.0004(7)	0.0000(6)	-0.0003(6)

The Temperature Factor has the Form of Exp(-T) Where
T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms
T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms.
Astar (i) [18] are Reciprocal Axial Lengths a h(i) are the Reflection Indices.

Table 6: Bond Angles (Degrees).

O5-Mn1-O11	90.59(5)	O12_b-Mn2-O31	89.55(5)
O5-Mn1-O21	95.83(5)	O12_b-Mn2-O41	170.83(5)
O5-Mn1-O5_c	180	O8-Mn3-O42	84.14(5)
O5-Mn1-O11_c	89.41(5)	O8-Mn3-O32_a	89.65(5)
O5-Mn1-O21_c	84.17(5)	O8-Mn3-O8_d	180
O11-Mn1-O21	95.89(5)	O8-Mn3-O42_d	95.86(5)
O5_c-Mn1 -O11	89.41(5)	O8-Mn3-O32_e	90.35(5)
O11-Mn1-O11_c	180	O32_a-Mn3-O42	96.02(5)
O11-Mn1-O21_c	84.11(5)	O8_d-Mn3-O42	95.86(5)
O5_c-Mn1-O21	84.17(5)	O42-Mn3-O42_d	180
O11_c-Mn1-O21	84.11(5)	O32_e-Mn3-O42	83.99(5)
O21-Mn1-O21_c	180	O8_d-Mn3-O32_a	90.35(5)
O5_c-Mn1-O11_c	90.59(5)	O32_a-Mn3-O42_d	83.99(5)
O5_c-Mn1-O21_c	95.83(5)	O32_a-Mn3-O32_e	180
O11_c-Mn1-O21_c	95.89(5)	O8_d-Mn3-O42_d	84.14(5)
O6-Mn2-O7	175.83(5)	O8_d-Mn3-O32_e	89.65(5)
O6-Mn2-O22	88.32(5)	O32_e-Mn3-O42_d	96.02(5)
O6-Mn2-O31	100.32(5)	Mn1-O11-C17	124.07(11)
O6-Mn2-O41	88.68(5)	Mn2_a-O12-C17	129.03(12)
O6-Mn2-O12_b	82.63(5)	Mn1-O21-C27	134.96(12)
O7-Mn2-O22	88.45(5)	Mn2-O22-C27	127.21(11)
O7-Mn2-O31	82.76(5)	Mn2-O31-C37	128.80(12)
O7-Mn2-O41	88.25(5)	Mn3_b-O32-C37	124.12(11)
O7-Mn2-O12_b	100.28(5)	Mn2-O41-C47	127.52(11)
O22-Mn2-O31	170.65(5)	Mn3-O42-C47	135.00(12)
O22-Mn2-O41	81.62(5)	H5A-O5-H5B	104(2)
O12_b-Mn2-O22	95.16(5)	Mn1-O5-H5B	125.9(15)
O31-Mn2-O41	94.89(5)	Mn1-O5-H5A	123.2(15)
Mn2-O6-H6B	130.4(15)	O21-C27-O22	124.01(17)
Mn2-O6-H6A	116.8(15)	O21-C27-C21	117.71(16)
H6A-O6-H6B	104.9(19)	O22-C27-C21	118.28(16)
Mn2-O7-H7B	130.0(15)	C36-C31-C37	121.02(18)
Mn2-O7-H7A	118.0(16)	C32-C31-C36	119.55(19)
H7A-O7-H7B	106(2)	C32-C31-C37	119.44(18)
Mn3-O8-H8B	122.0(15)	C31-C32-C33	120.0(2)
H8A-O8-H8B	105(2)	C32-C33-C34	120.2(2)
Mn3-O8-H8A	128.5(15)	C33-C34-C35	120.1(2)
C12-C11-C16	119.48(19)	C34-C35-C36	120.4(2)

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C16-C11-C17	120.94(17)	C31-C36-C35	119.8(2)
C12-C11-C17	119.58(18)	O31-C37-O32	123.38(17)
C11-C12-C13	119.9(2)	O31-C37-C31	118.53(16)
C12-C13-C14	120.3(2)	O32-C37-C31	118.09(16)
C13-C14-C15	120.0(2)	C42-C41-C47	120.52(17)
C14-C15-C16	120.4(2)	C46-C41-C47	119.83(18)
C11-C16-C15	119.9(2)	C42-C41-C46	119.66(19)
O12-C17-C11	118.67(16)	C41-C42-C43	120.1(2)
O11-C17-C11	118.01(16)	C42-C43-C44	120.1(2)
O11-C17-O12	123.32(17)	C43-C44-C45	120.2(2)
C22-C21-C27	120.52(17)	C44-C45-C46	120.3(2)
C22-C21-C26	119.46(19)	C41-C46-C45	119.7(2)
C26-C21-C27	120.02(18)	O41-C47-C41	118.18(16)
C21-C22-C23	120.0(2)	O42-C47-C41	117.76(16)
C22-C23-C24	120.3(2)	O41-C47-O42	124.06(17)
C23-C24-C25	120.1(2)	C11-C12-H12	120
C24-C25-C26	120.3(2)	C13-C12-H12	120
C21-C26-C25	119.8(2)	C12-C13-H13	120
C14-C13-H13	120	C32-C33-H33	120
C13-C14-H14	120	C34-C33-H33	120
C15-C14-H14	120	C33-C34-H34	120
C14-C15-H15	120	C35-C34-H34	120
C16-C15-H15	120	C34-C35-H35	120
C11-C16-H16	120	C36-C35-H35	120
C15-C16-H16	120	C31-C36-H36	120
C21-C22-H22	120	C35-C36-H36	120
C23-C22-H22	120	C41-C42-H42	120
C22-C23-H23	120	C43-C42-H42	120
C24-C23-H23	120	C42-C43-H43	120
C23-C24-H24	120	C44-C43-H43	120
C25-C24-H24	120	C43-C44-H44	120
C24-C25-H25	120	C45-C44-H44	120
C26-C25-H25	120	C44-C45-H45	120
C21-C26-H26	120	C46-C45-H45	120
C25-C26-H26	120	C41 -C46-H46	120
C31-C32-H32	120	C45-C46-H46	120
C33-C32-H32	120		

Table 7: Translation of Symmetry Code to Equiv.Pos.

a =	[1455.00] =	[1_455] =	-1+x, y,z
b =	[1655.00] =	[1_655] =	1+x, y,z
c =	[2556.00] =	[2_556] =	-x, -y,1-z
d =	[2566.00] =	[2_566] =	-x,1-y,1-z
e =	[2666.00] =	[2_666] =	1-x,1-y,1-z

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f =	[2656.00] =	[2_656] =	1-x, -y,1-z
g =	[2655.00] =	[2_655] =	1-x, -y, -z
h =	[2667.00] =	[2_667] =	1-x,1-y,2-z
i =	[1454.00] =	[1_454] =	-1+x, y, -1+z
j =	[1554.00] =	[1_554] =	x, y, -1+z
k =	[1656.00] =	[1_656] =	1+x, y,1+z
l =	[1556.00] =	[1_556] =	x, y,1+z

Table 8: Formal Single Bonds.

C4-C4 1.54	C4-C3 1.52	C4-C2 1.46	C4-N3 1.47	C4-N2 1.47	C4-O2 1.43
C3-C3 1.46	C3-C2 1.45	C3-N3 1.40	C3-N2 1.40	C3-O2 1.36	C2-C2 1.38
C2-N3 1.33	C2-N2 1.33	C2-O2 1.36	N3-N3 1.45		
N3-N2 1.45	N3-O2 1.36	N2-N2 1.45	N2-O2 1.41		

Table 9: Formal double bonds.

C3-C3 1.34	C3-C2 1.31	C3-N2 1.32	C3-O1 1.22	C2-C2 1.28	C2-N2 1.32
C2-O1 1.16	N3-O1 1.24	N2-N2 1.25	N2-O1 1.21		

Table 10: Formal triple bonds (Aromatic bonds).

C2-C2 1.20	C2-N1 1.16	C3-C3 1.40	C2-N2 1.34	N2-N2 1.35	
C4-C4 1.54	C4-C3 1.52	C4-C2 1.46	C4-N3 1.47	C4-N2 1.47	C4-O2 1.43
C3-C3 1.46	C3-C2 1.45	C3-N3 1.40	C3-N2 1.40	C3-O2 1.36	C2-C2 1.38
C2-N3 1.33	C2-N2 1.33	C2-O2 1.36	N3-N3 1.45	N3-N2 1.45	N3-O2 1.36
N2-N2 1.45	N2-O2 1.41				

Table 11: Contact Distances (Å).

Mn1	. O12	3.8473(14)	Mn2	.H5A_b	3.402(18)
Mn1	. O22	3.5720(14)	Mn2	.H8B_e	3.404(18)
Mn1	.C11	3.8382(19)	Mn3	.H6A_a	3.330(17)
Mn1	.C12	3.985(2)	Mn3	.H6B	3.329(17)
Mn1	. O22_c	3.5720(14)	Mn3	.H6A_e	3.330(18)
Mn1	.C11_c	3.8382(19)	Mn3	.H6B_d	3.329(17)
Mn1	. O12_c	3.8473(14)	O5	. O11	3.097(2)
Mn1	.C12_c	3.985(2)	O5	. O21	3.223(2)
Mn2	.C46	4.041(2)	O5	. O22	3.117(2)
Mn2	. O11_b	3.4526(14)	O5	.O31_a	2.8471(19)
Mn2	.O32	3.4453(13)	O5	.O41	2.8449(19)
Mn2	. C21	3.910(2)	O5	.O11_c	3.065(2)
Mn2	. C26	4.032(2)	O5	.O21_c	2.911(2)
Mn2	. C41	3.923(2)	O6	.O12_b	2.886(2)
Mn3	. C32_a	3.979(2)	O6	.O22	3.038(2)
Mn3	.O31_e	3.8492(14)	O6	.O32	3.078(2)
Mn3	.O31_a	3.8492(14)	O6	.O41	3.050(2)
Mn3	.O41	3.5731(14)	O6	.O32_e	2.8243(19)
Mn3	. C31_a	3.8329(19)	O6	.O42_e	2.9009(19)
Mn3	. C32_e	3.979(2)	O7	.O11_b	3.086(2)
Mn3	. O41_d	3.5731(14)	O7	.O22	3.040(2)

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Mn3	.C31_e	3.8329(19)	O7	.O31	2.884(2)
Mn1	.H7A_a	3.342(18)	O7	.O41	3.037(2)
Mn1	.H7B_c	3.322(17)	O7	.O11_c	2.8281(19)
Mn1	.H7B	3.322(17)	O7	.O21_f	2.8978(19)
Mn1	.H7A_f	3.342(18)	O8	.O32_a	3.0715(19)
Mn2	.H5B	3.283(17)	O8	.O42	2.9104(19)
Mn2	.H8A_d	3.295(17)	O8	.O12_d	2.8488(19)
O8	.O22_d	2.8390(19)	O22	.O5	3.117(2)
O8	.O32_e	3.090(2)	O22	.O8_d	2.8390(19)
O8	.O41_d	3.119(2)	O22	.O12_b	3.2197(18)
O8	.O42_d	3.225(2)	O22	.C26	2.802(3)
O11	.Mn2_a	3.4526(14)	O22	.O41	2.845(2)
O11	.O5	3.097(2)	O22	.Mn1	3.5720(14)
O11	.O7_a	3.086(2)	O22	.O7	3.040(2)
O11	.O21	3.2241(18)	O31	.O12_b	3.075(2)
O11	.C12	2.795(3)	O31	.Mn3_b	3.8492(14)
O11	.O7_c	2.8281(19)	O31	.C46	3.378(3)
O11	.O21_c	2.909(2)	O31	.Mn3_b	3.8492(14)
O11	.O5_c	3.065(2)	O31	.O5_b	2.8471(19)
O12	.O6_a	2.886(2)	O31	.O7	2.884(2)
O12	.O22_a	3.2197(18)	O31	.O41	3.2107(18)
O12	.C26_a	3.367(3)	O31	.C36	2.836(3)
O12	.Mn1	3.8473(14)	O32	.O6	3.078(2)
O12	.C16	2.838(3)	O32	.O42_b	3.2294(19)
O12	.O31_a	3.075(2)	O32	.O42_e	2.907(2)
O12	.O8_d	2.8488(19)	O32	.Mn2	3.4453(13)
O21	.C22	2.800(3)	O32	.C32	2.793(3)
O21	.O11	3.2241(18)	O32	.O8_b	3.0715(19)
O21	.O7_f	2.8978(19)	O32	.O8_e	3.090(2)
O21	.O5	3.223(2)	O32	.O6_e	2.8243(19)
O21	.O5_c	2.911(2)	O41	.O5	2.8449(19)
O21	.C12	3.396(3)	O41	.O8_d	3.119(2)
O21	.O11_c	2.909(2)	O41	.C46	2.797(3)
O21	.C11	3.404(2)	O41	.O7	3.037(2)
O22	.O6	3.038(2)	O41	.Mn3	3.5731(14)
O41	.O6	3.050(2)	O41	.H46	2.5
O41	.O31	3.2107(18)	O42	.H42	2.51
O41	.O22	2.845(2)	O42	.H6A_e	2.079(19)
O42	.O8	2.9104(19)	C11	.Mn1	3.8382(19)
O42	.C31_a	3.401(2)	C11	.O21	3.404(2)
O42	.O32_a	3.2294(19)	C11	.C14	2.779(3)
O42	.O8_d	3.225(2)	C11	.C25_a	3.557(3)
O42	.O6_e	2.9009(19)	C11	.C26_a	3.544(3)
O42	.C42	2.800(3)	C11	.C27	3.438(2)

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O42	.C32_a	3.395(3)	C12	.Mn1	3.985(2)
O42	.O32_e	2.907(2)	C12	.O11	2.795(3)
O11	.H12	2.5	C12	.O21	3.396(3)
O11	.H7A_a	2.65(3)	C12	.C15	2.768(3)
O11	.H7B_c	1.991(18)	C12	.C23_a	3.537(3)
O12	.H8B_d	2.01(2)	C13	.C16	2.767(3)
O12	.H16	2.56	C13	.C22	3.377(3)
O21	.H22	2.51	C14	.C11	2.779(3)
O21	.H7A_f	2.07(2)	C15	.C12	2.768(3)
O22	.H5B	2.64(3)	C15	.C26	3.535(3)
O22	.H8A_d	2.001(19)	C16	.O12	2.838(3)
O22	.H26	2.51	C16	.C13	2.767(3)
O31	.H36	2.56	C16	.C25_a	3.361(3)
O31	.H5A_b	2.01(2)	C17	.O5	3.415(2)
O32	.H32	2.5	C17	.C21_a	3.455(2)
O32	.H6A	2.60(3)	C17	.C26_a	3.554(3)
O32	.H6B_e	1.985(18)	C21	.C24	2.775(3)
O41	.H5B	2.016(19)	C21	.Mn2	3.910(2)
O41	.H8A_d	2.68(3)	C21	.C17_b	3.455(2)
C22	.O21	2.800(3)	C32	.O32	2.793(3)
C22	.C13	3.377(3)	C32	.O42_b	3.395(3)
C22	.C25	2.765(3)	C32	.Mn3_b	3.979(2)
C23	.C12_b	3.537(3)	C33	.C42_b	3.369(3)
C23	.C26	2.766(3)	C33	.C36	2.767(3)
C24	.C21	2.775(3)	C34	.C31	2.775(3)
C25	.C16_b	3.361(3)	C34	.C42_b	3.581(3)
C25	.C22	2.765(3)	C35	.C46_b	3.523(3)
C25	.C11_b	3.557(3)	C35	.C32	2.766(3)
C26	.O12_b	3.367(3)	C36	.O31	2.836(3)
C26	.Mn2	4.032(2)	C36	.C33	2.767(3)
C26	.C11_b	3.544(3)	C36	.C45	3.381(3)
C26	.C17_b	3.554(3)	C37	.C41	3.460(2)
C26	.C23	2.766(3)	C37	.C46	3.563(3)
C26	.C15	3.535(3)	C37	.O8_e	3.410(2)
C26	.O22	2.802(3)	C41	.Mn2	3.923(2)
C27	.O7	3.364(2)	C41	.C37	3.460(2)
C27	.C11	3.438(2)	C41	.C44	2.773(3)
C31	.C34	2.775(3)	C42	.C34_a	3.581(3)
C31	.O42_b	3.401(2)	C42	.C33_a	3.369(3)
C31	.Mn3_b	3.8329(19)	C42	.C45	2.763(3)
C31	.C45	3.577(3)	C42	.O42	2.800(3)
C31	.C46	3.545(3)	C43	.C32	3.546(3)
C31	.Mn3_b	3.8329(19)	C43	.C46	2.768(3)
C31	.C47_b	3.443(2)	C44	.C41	2.773(3)
C32	.Mn3_b	3.979(2)	C45	.C42	2.763(3)

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C32	.C43	3.546(3)	C45	.C36	3.381(3)
C32	.C35	2.766(3)	C45	.C31	3.577(3)
C46	.C31	3.545(3)	H5A	.O31_a	2.01(2)
C46	.Mn2	4.041(2)	H5A	.C37_a	2.70(2)
C46	.C43	2.768(3)	H5A	.H36_a	2.52
C46	.C35_a	3.523(3)	H5B	.Mn2	3.283(17)
C46	.C37	3.563(3)	H5B	.O22	2.64(3)
C46	.O41	2.797(3)	H5B	.O41	2.016(19)
C46	.O31	3.378(3)	H5B	.C47	2.98(2)
C47	.C31_a	3.443(2)	H5B	.H8A_d	2.54(4)
C47	.O6	3.379(2)	H6A	.Mn3_b	3.330(17)
C17	.H16	2.68	H6A	.O32	2.60(3)
C17	.H12	2.65	H6A	.Mn3_b	3.330(17)
C17	.H7B_c	2.97(2)	H6A	.O42_e	2.079(19)
C17	.H8B_d	2.71(2)	H6A	.C47_e	2.74(2)
C24	.H23_g	3.05	H6B	.Mn3	3.329(17)
C27	.H7A_f	2.73(2)	H6B	.O32_e	1.985(18)
C27	.H26	2.66	H6B	.C37_e	2.95(2)
C27	.H8A_d	2.95(2)	H7A	.Mn1_b	3.342(18)
C27	.H22	2.67	H7A	.O11_b	2.65(3)
C34	.H43_h	3.06	H7A	.Mn1_f	3.342(18)
C37	.H32	2.64	H7A	.O21_f	2.07(2)
C37	.H36	2.68	H7A	.C27_f	2.73(2)
C37	.H5A_b	2.70(2)	H7A	.H22_f	2.57
C37	.H6B_e	2.95(2)	H7B	.Mn1	3.322(17)
C47	.H5B	2.98(2)	H7B	.O11_c	1.991(19)
C47	.H42	2.66	H7B	.C17_c	2.97(2)
C47	.H46	2.66	H8A	.Mn2_d	3.295(17)
C47	.H6A_e	2.74(2)	H8A	.O22_d	2.001(18)
H5A	.Mn2_a	3.402(18)	H8A	.O41_d	2.68(3)
H8A	.C27_d	2.95(2)	H23	.C24_g	3.05
H8A	.H5B_d	2.54(4)	H23	.H45_f	2.5
H8B	.Mn2_e	3.404(18)	H24	.H23	2.32
H8B	.O12_d	2.01(2)	H24	.H25	2.32
H8B	.C17_d	2.71(2)	H24	.H35_j	2.53
H8B	.H16_d	2.51	H25	.H24	2.32
H12	.O11	2.5	H25	.H26	2.34
H12	.C17	2.65	H25	.H43_e	2.52
H12	.H13	2.34	H26	.O22	2.51
H13	.H12	2.34	H26	.C27	2.66
H13	.H14	2.32	H26	.H25	2.34
H13	.H35_f	2.52	H32	.O32	2.5
H14	.H13	2.32	H32	.C37	2.64
H14	.H15	2.32	H32	.H33	2.34
H15	.H14	2.32	H33	.H32	2.34

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H15	.H16	2.34	H33	.H34	2.33
H15	.H34_i	2.55	H33	.H15_e	2.5
H15	.H33_e	2.5	H34	.H15_k	2.55
H16	.O12	2.56	H34	.H33	2.33
H16	.C17	2.68	H34	.H35	2.32
H16	.H15	2.34	H35	.H24_l	2.53
H16	.H8B_d	2.51	H35	.H34	2.32
H22	.O21	2.51	H35	.H36	2.34
H22	.C27	2.67	H35	.H13_f	2.52
H22	.H23	2.33	H36	.O31	2.56
H22	.H7A_f	2.57	H36	.C37	2.68
H23	.H22	2.33	H36	.H5A_b	2.52
H23	.H24	2.32	H36	.H35	2.34
H42	.O42	2.51	H44	.H45	2.32
H42	.C47	2.66	H45	.H44	2.32
H42	.H43	2.34	H45	.H46	2.34
H43	.H42	2.34	H45	.H23_f	2.5
H43	.H44	2.32	H46	.O41	2.5
H43	.C34_h	3.06	H46	.C47	2.66
H43	.H25_e	2.52	H46	.H45	2.34
H44	.H43	2.32			

Photoluminescence spectrum Mn-MOF

The luminescence spectrum of Mn-MOF was measured in the range 200-800nm, utilizing PerkinELmer Luminescence Spectrophotometer by absorption and emission modes.

Results and Discussion

Structural commentary

The asymmetric unit consists of three [19] Mn^{II}, two water molecules, and four carboxylate anions. The Mn^{II} is six-coordinated with octahedral geometry by six oxygen atoms. The apical position of Mn1 is occupied by two oxygen atoms at O22-Mn-O22 angle of 180.00 with a contact distance of 2.1635(13). The apical positions of Mn2 are occupied by two oxygen atoms at O22-Mn2-O31 angle of 89.95(5) with a contact distance of 2.1754(14): 2.1802(14). The apical positions of Mn3 are occupied by two oxygen atoms at O33-Mn-O33 angle of 180.00 with a contact distance of 2.1792(13). Two adjacent Mn^{II} ions are connected by two carboxylic oxygen atoms to form $[Mn_2O_2]$ ring with Mn1...Mn2 distances of 2.16Å and Mn2...Mn3 of distances of 2.18 Å, respectively forming a 3D framework with two types of channels (Figure 2a). Figure 2b is the ball and stick illustration of Mn-MOF displaying hydrogen bonding system.

Supramolecular features

Figure 3 shows the crystal packing of Mn-MOF with the molecules linked into a three-dimensional network via intermolecular C–H...O, C–H...N, O –H...O, and N–H...O hydrogen bonds (Tables 12 & 13).

Table 12: Hydrogen-bond geometry (Å°).

D - H	D... A	D - H... A	A... H... A*	A'...H..A"	H... A
O5 -- H5A ... O31	0.84(2)	2.01(2)	2.8471(19)	177(2)	[1455.01]
O5 -- H5B ... O41	0.840(19)	2.016(19)	2.8449(19)	169(2)	[2556.01]
O6 -- H6A ... O32	0.841(18)	2.60(3)	3.078(2)	117(2)	[2566.01]
O6 -- H6A ... O42	0.841(18)	2.079(19)	2.9009(19)	166(2)	[2666.01]
O6 -- H6B ... O32	0.841(18)	1.985(18)	2.8243(19)	176(2)	[2666.01]
O7 -- H7A ... O21	0.843(18)	2.07(2)	2.8978(19)	169(2)	[2656.01]
O7 -- H7B ... O11	0.839(18)	1.991(19)	2.8281(19)	175.6(17)	[2556.01]
O8 -- H8A ... O22	0.843(18)	2.001(18)	2.8390(19)	173(2)	[2566.01]
O8 -- H8B ... O12	0.843(19)	2.01(2)	2.8488(19)	173(2)	[2566.01]

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Table 13: Translation Code and Equivalent Position.

[1455.]	=	[1_455]	=	-1+x, y,z
[2556.]	=	[2_556]	=	-x, -y,1-z
[2566.]	=	[2_566]	=	-x,1-y,1-z
[2666.]	=	[2_666]	=	1-x,1-y,1-z
[2656.]	=	[2_656]	=	1-x, -y,1-z

Refinement details

Table 12 & 13 shows the hydrogen and oxygen and hydrogen bound atoms were refined as O--H..O = 0.839(18) to 0.843(19); A'...H...A" = 117(2) to 177(2).The rest of the hydrogen atoms were calculated geometrically and refined with a riding model U(eq) = 1/3 of the trace of the orthogonalized U Tensor with bond lengths of C–H being 0.95 Å(see Table 2).

Special geometric details

All the estimated standard deviations (esds), except the esds in the dihedral [20] angle between two l.s. [21] planes were calculated using the total covariance matrix. An isotropic treatment [22] of cell esds was employed for esds estimated standard deviations involving l.s [23] planes. The cell estimated standard deviations considered in this work were treated individually within the esds in distances [24], angles and torsion angles and correlations in cell parameters outlined by the crystal symmetry (Table 3,6 & 11). The coordination mode of manganese (II) with 1,10 phenanthroline and carboxylic acids was determined, results showing octahedral geometry [7,8]. Bond distances and angles, selected bond lengths (Angstrom), identification of chiral center(s) and their (R/S)-configuration were evaluated, and results shown in Tables 2-6 [9,25].

Photoluminescence studies of Mn-MOF

Figure 4 shows the fluorescence intensity of Mn-MOF at 308 nm increased with increase in adsorption time. The investigation of the luminescence properties of this compound revealed its efficient room-temperature phosphorescence in solution with a remarkable weak quenching by molecular oxygen [26-35]. The photophysical result displayed how the electron donor ability of the ligands and the electron–withdrawing character of the manganese(II) results in bathochromic shift of emission maximum (in the 324-460nm) and a decrease in the luminescence quantum yield showing the Mn(II) play a key role in the observed phosphorescence [5,6].

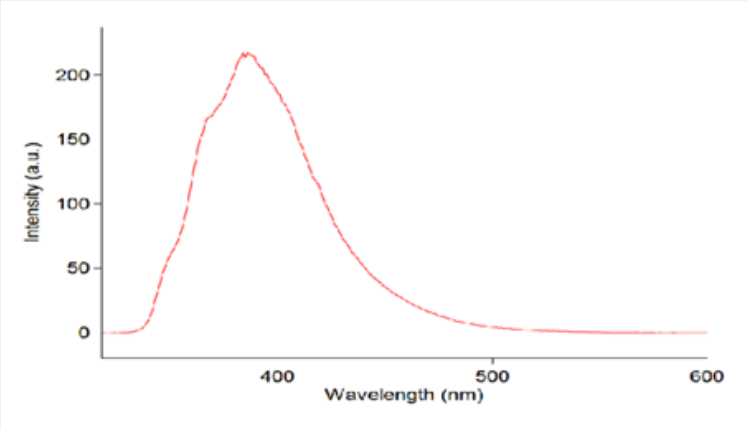

Figure 4: Shows photoluminescence spectrum of Mn-MOF.

Conclusion

A new Mn(II) compound has been synthesized by our group. The structural arrangement within this compound shows define pores for accommodating other molecules by cation substitution. The investigation of the luminescence properties of Mn- MOF reveals efficient room-temperature phosphorescence in solution with a remarkable weak quenching by molecular oxygen. The pores in the Mn-MOF structure and photophysical results displayed in the observed phosphorescence is an indication that this compound can be used in fields such as drugs industries, as luminescence sensors to analyze water, air, and chemical pollutions. The correlation of the porosity and luminescence activity should be taken into account for designing new potential catalytic and energy storage materials.

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