Supplementary materials

Synthesis of New Homopiperazine-1.4-Diium Tetrachloridromercurate (II) Monohydrate $(C_5H_{14}N_2)[HgCl_4]\cdot H_2O$, Crystal Structure, Hirshfeld Surface, Spectroscopy, Thermal Analysis, Antioxidant Activity, Electric and Dielectric Behavior

Chaima Ayari [1], Abdullah A. Alotaibi [2,*], Mohammed A. Baashen [2], Khalid M. Alotaibi [3], Khadijah H. Alharbi [4], Abdelhak Othmani [5], Wataru Fugita [6], Cherif Ben Nasr [1] and Mohamed Habib Mrad [1,2]

[1] Materials Chemistry Laboratory, Faculty of Sciences of Bizerte, University of Carthage, Zarzouna 7021, Tunisia; ayarichaima33@gmail.com (C.A.); cherif_bennasr@yahoo.fr (C.B.N.); m.mrad@su.edu.sa (M.H.M.)
[2] Department of Chemistry, College of Sciences and Humanities, Shaqra University, Shaqra 11911, Saudi Arabia; mbaashen@su.edu.sa
[3] Department of Chemistry College of Science, King Saud University, Riyadh 11451, Saudi Arabia; khalid.m@ksu.edu.sa
[4] Department of Chemistry, College of Sciences & Arts, King Abdulaziz University, Rabigh 21589, Saudi Arabia; khalharbe@kau.edu.sa
[5] Laboratory of Material Physics: Structures and Properties, LR01 ES15, Faculty of Sciences, University of Carthage, Zarzouna 7021, Tunisia; othmaniabdelhak1687@gmail.com
[6] Department of Marine Electronics and Mechanical Engineering, Faculty of Marine Engineering, Tokyo University of Marine Science and Technology, Tokyo 135-8533, Japan; fujitaw@st.seikei.ac.jp
* Correspondence: aaalotaibi@su.edu.sa

Table S1. The different H-Bonds present in $(C_5H_{14}N_2)[HgCl_4]\cdot H_2O$.

D—H…*A*	D—H (Å)	H…*A* (Å)	D…*A* (Å)	D—H…*A* (°)
C1—H1*C*…Cl3^{i}	0.97	2.92	3.558 (6)	124
C1—H1*D*…Cl3^{ii}	0.97	2.85	3.484 (7)	124
C2—H2*D*…Cl3^{iii}	0.97	2.89	3.606 (7)	132
C3—H3*A*…Cl4	0.97	2.85	3.802 (7)	168
C3—H3*B*…Cl2^{v}	0.97	2.75	3.510 (7)	136
C5—H5*A*…Cl2^{v}	0.97	2.85	3.505 (7)	126
C5—H5*B*…Cl1^{v}	0.97	2.9	3.807 (7)	156
N1—H1*A*…O1^{vi}	0.89	1.86	2.744 (7)	171
N1—H1*B*…Cl1^{iii}	0.89	2.8	3.348 (5)	121
N1—H1*B*…Cl4^{vi}	0.89	2.55	3.216 (5)	133
N2—H2*A*…Cl1	0.89	2.44	3.223 (6)	147
N2—H2*B*…Cl2^{ii}	0.89	2.3	3.104 (5)	149
N2—H2*B*…Cl3^{i}	0.89	2.95	3.424 (6)	115
O1—H1*P*…Cl2	0.8	2.46	3.209 (5)	156
O1—H1*O*…Cl1	0.8	2.54	3.309 (5)	162

Symmetry codes: (i) –x,y+1/2,–z+1/2; (ii) –x+1, y+1/2, –z+1/2 ; (iii) x, –y+3/2, z+1/2 ; (iv) –x, –y+1, –z+1 ; (v) x–1, y, z ; (vi) x–1, –y+3/2, z+1/2 ; (vii) –x+1, –y+1, –z+1.

Table S2. The different distances and angles of every part in $(C_5H_{14}N_2)[HgCl_4]\cdot H_2O$.

Distances (Å)		Angles (°)	
		$[HgCl_4]^{2-}$	
Hg1—Cl1	2.582 (2)	Cl4—Hg1—Cl3	137.77 (7)
Hg1—Cl2	2.654 (2)	Cl4—Hg1—Cl1	106.74 (6)

Hg1—Cl3	2.4135 (19)	Cl3—Hg1—Cl1	105.51 (5)
Hg1—Cl4	2.401 (2)	Cl4—Hg1—Cl2	96.65 (5)
		Cl3—Hg1—Cl2	105.58 (5)
		Cl1—Hg1—Cl2	97.23 (5)
$(C_5H_{14}N_2)^{2+}$			
C1—N2	1.473 (7)	N2—C1—C2	113.7 (5)
C1—C2	1.518 (8)	N1—C2—C1	113.1 (5)
C2—N1	1.481 (7)	C4—C3—N1	112.8 (5)
C3—C4	1.514 (8)	C3—C4—C5	116.5 (6)
C3—N1	1.519 (8)	N2—C5—C4	115.7 (5)
C4—C5	1.515 (9)	C2—N1—C3	115.6 (5)
C5—N2	1.502 (8)	C1—N2—C5	119.7 (5)
H_2O			
O1—H1P	0.7999	H1P—O1—H1O	104.9
O1—H1O	0.8016		

Table S3. The main bands detected in the infrared spectrum of $(C_5H_{14}N_2)[HgCl_4]\cdot H_2O$: Wavenumbers values and their modes of vibration.

Detected	Assignment	Detected	Assignment
3522	ν (O–H)	1225	ν_{as} (C–N)
3433		1125	
3127	ν_{as} (N–H)	1068	ν_{as} (C–C)
3012	ν_s(N–H)		
2840	ν_s (C–H)	979	ϱ(NH_2)
2776	ν_{as}(C–H)		
1625	δ (NH_2)	883	δ (C–C–C)
	δ (H_2O)	829	δ (C–C–N)
1572	δ_{as} (C–N–H)	531	δ (C–N–C)
1456	δ (CH_2)		

ν: Stretching; δ: Bending; ϱ: Rocking; as: asymmetric; s: symmetric.