crystals

MDPI

Article

Physico-chemical characterization, DFT Modeling and biological Activities of a new Zn (II) complex containing melamine as a template

Thouraya Salah[1], Noureddine Mhadhbi[2], Ali Ben Ahmed[3], Besma Hamdi[1], Najeh Krayem[4], Mohamed Loukil[1], Ahlem Guesmi[5], Lotfi Khezami[5], Ammar Houas[6], Naoufel Ben Hamadi[5], Houcine Naïli[2]* and Ferdinando Costantino[7]*

[1]*Laboratory of Materials Science and Environment, Faculty of Sciences of Sfax, University of Sfax, Tunisia.*

[2]*Laboratory Physico Chemistry of the Solid State, Department of Chemistry, Faculty of Sciences, University of Sfax, BP 1171, 3000 Sfax, Tunisia.*

[3]*Laboratory of Applied Physics, University of Sfax, Faculty of Sciences, Sfax, Tunisia.*

[4]*Laboratory of Biochemistry and Enzymatic Engineering of Lipases, University of Sfax, National School of Engineering of Sfax (ENIS), Tunisia.*

[5]*Chemistry Department, College of Science, IMSIU (Imam Mohammad Ibn Saud Islamic University), P.O. Box 5701, Riyadh 11432, Saudi Arabia.*

[6]*Research Laboratory of Catalysis and Materials for Environment and Processes, University of Gabes, City RiadhZerig, Gabes, 6029, Tunisia.*

[7]*Department of Chemistry Biology and Biotechnologies University of Perugia Via Elce di Sotto 8, 06123 Perugia, Italy.*

* Correspondence: Ferdinando Costantino : E-mail: ferdinando.costantino@unipg.it

Table S1. Observed and calculated bond lengths (Å) and angles (°) of $[ZnCl_4]^{2-}$ tetrahedron.

		WB97XD/Lanl2dz		CAM-B3LYP/Lanl2dz	
Parameters	**Exp.**	**DFT**	**Δ (%)**	**DFT**	**Δ (%)**
Bond length (Å)					
Zn1-Cl5	2.2332 (13)	2.31486	3.52	2.33535	4.37
Zn1-Cl2	2.2716 (13)	2.35524	3.55	2.33829	2.85
Zn1-Cl3	2.2799 (13)	2.36775	3.71	2.36991	3.79
Zn1-Cl4	2.2827 (13)	2.47959	7.94	2.41215	5.36
Bond angle (°)					
Cl2-Zn1-Cl3	107.12 (5)	99.56	7.05	102.43	4.37
Cl2-Zn1-Cl4	108.73 (5)	102.41	5.81	106.81	1.79
Cl3-Zn1-Cl4	107.41 (5)	102.26	4.79	106.12	1.20
Cl5-Zn1-Cl2	111.29 (5)	119.63	6.97	115.61	3.73
Cl5-Zn1-Cl3	109.81 (5)	107.25	2.33	107.55	2.05
Cl5- Zn1-Cl4	112.27 (6)	121.46	7.56	117.08	4.10

Table S2. Observed and calculated bond length (Å) and bond angles (°) of the compound $(C_3H_7N_6)_2[ZnCl_4]\cdot H_2O$.

		WB97XD/Lanl2dz		CAM-B3LYP/Lanl2dz	
Parameters	**Exp.**	**DFT**	**Δ (%)**	**DFT**	**Δ (%)**
Bond length (Å)					
N1-C4	1.356 (5)	1.361	0.36	1.361	0.36
N1-C15	1.357 (5)	1.381	1.73	1.379	1.60
N2-C10	1.356 (5)	1.360	0.29	1.357	0.07
N2-C12	1.361 (5)	1.383	1.59	1.380	0.58
N3-C4	1.336 (6)	1.340	0.29	1.339	0.22
N3-C16	1.338 (5)	1.343	0.37	1.344	0.44
N7-C12	1.363 (6)	1.377	1.01	1.355	0.58
N7-C11	1.398 (6)	1.362	2.57	1.374	1.71
N8-C11	1.340 (5)	1.343	0.22	1.346	0.44
N8-C10	1.340 (5)	1.339	0.07	1.335	0.37
N18-C12	1.478 (6)	1.335	9.67	1.435	2.90
N13-C15	1.362 (6)	1.360	0.14	1.367	0.36
N13-C16	1.403 (6)	1.379	1.71	1.385	1.28
N14-C16	1.487 (6)	1.338	10.02	1.452	2.35
N19-C15	1.483 (6)	1.348	9.10	1.465	1.22
Bond angle (°)					
N1-C15-N13	118.1 (4)	117.25	0.72	119.2	0.92
N1-C15-N19	117.5 (4)	117.04	0.39	117.9	0.34
N2-C12-N7	117.0 (4)	120.62	3.00	120.1	2.58

N2-C12-N18	117.3 (4)	118.34	0.87	118.4	0.9
N3-C4-N1	121.3 (4)	120.69	0.50	122.2	0.73
N3-C16-N13	122.3 (4)	125.69	2.69	125.2	2.31
N3-C16-N14	117.6 (4)	120.32	2.26	116.6	0.85
C4-N1-C15	121.9 (4)	121.95	0.041	120.15	1.43
C4-N3-C16	118.0 (4)	117.20	0.67	116.20	1.52
N5-C10-N2	119.2 (4)	118.32	0.73	117.85	1.13
N5-C10-N8	119.1 (4)	120.61	1.25	117.65	1.21
N6-C4-N1	119.1 (4)	120.23	0.94	118.13	0.81
C10-N2-C12	121.8 (4)	122.46	0.53	119.52	1.87
C11-N8-C10	118.0 (4)	118.80	0.67	117.30	0.59
C12-N7-C11	120.1 (4)	118.75	1.12	117.60	2.08
N13-C16-N14	120.1 (4)	120.28	0.15	119.88	0.18
N13-C15-N19	124.4 (4)	125.61	0.96	123.20	0.96
C15-N13-C16	118.3 (4)	119.57	1.06	117.24	0.89
N7-C11-N17	122.4 (4)	122.00	0.32	121.06	1.09
N7-C12-N18	125.6 (4)	124.81	0.62	122.74	2.27
N8-C10-N2	121.7 (4)	123.52	1.47	124.12	1.95
N8-C11-N7	121.3 (4)	123.28	1.60	122.44	0.93
N8-C11-N17	116.3 (4)	117.71	1.19	117.3	0.85
N6-C4-N3	119.7 (4)	120.35	0.54	118.72	0.81

Table S3. Wavenumbers (cm^{-1}) and assignments, of the observed and calculated bands, in the Infrared (FT-IR) and Raman spectra of the title compound.

Experimental		**Theoretical**	**Theoretical**	**Assignments**
FT-IR	**Raman**	WB97XD/Lanl2dz	CAM-B3LYP/Lanl2dz	
3778	3793	3696	3795	ν_{as}(OH)
3689	3696	3608	3730-3673	$\nu_{as}(NH_2)$
3601	3636-3521	3546	3601-3502	$\nu_{s}(NH_2)$
3499	3491	3464	3497	ν_{s}(OH)
3372-3245	3387-3175	3439-3264	3469-3234	ν(NH)
1728-1677	1723-1717	1697	1735-1697	ν(C=N)
1633	1639	1621	1665	$\delta(H_2O)$
1519	1517	1551	1646-1521	$\delta(NH_2)$
1481-1341	1433-1337	1494	1510-1349	δ(C-N-C)
1252-1024	1323-1027	1385	1259-1020	$\delta(N\text{-}C\text{-}NH_2)$
980	979	998	985	δ(C-N-C) (ring)
814	931	928	863	ν(NH)
777	865	867	847	ν_{as}(NCN)
725	767	800	805	ν_{s}(NCN)

688	680	673	715-693	ν(NH)
618	617	629	624-581	ν(NH_2)
-	563	574	578	$\nu_{as}(ZnCl_4)$
-	465	387	469	$\nu_{s}(ZnCl_4)$
-	363	358	358	$\delta_{as}(ZnCl_4)$
-	237	251	246	$\delta_{s}(ZnCl_4)$

Table S4. Electric dipole moment, the polarizability, and second hyperpolarizability for $(C_3H_7N_6)_2[ZnCl_4]\cdot H_2O$.

Theoretical WB97XD/Lanl2dz		**Theoretical** CAM-B3LYP/Lanl2dz
Dipole moment ($\boldsymbol{D}$)		
μ_x	1.1274	0.3840
μ_y	10.4928	-9.0788
μ_z	-3.4779	-0.5113
μ_{tot}	1.1115	9.1013
Polarizability ($\times \boldsymbol{10^{-24}esu}$)		
α_{xx}	15.4051	11.3598
α_{yy}	26.7962	25.3044
α_{zz}	25.2154	26.3131
α_{xy}	0.3803	2.8974
α_{xz}	1.6946	1.0269
α_{yz}	1.8022	0.3272
α_{tot}	22.4722	20.9924
Second hyperpolarizability ($\times \boldsymbol{10^{-36}esu}$)		
γ_{xxxx}	4.5794	5.6500
γ_{yyyy}	1.5133	1.5671
γ_{zzzz}	1.1362	0.6439
γ_{xxyy}	1.0160	1.1265
γ_{xxzz}	1.0404	1.4214
γ_{yyzz}	0.4063	0.4449
$\langle\gamma\rangle$	2.4308	2.7693