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Synthesis, Characterization, and DFT Investigation of a Zinc(II)–Silver(I) Bimetallic Complex, $[Zn(Dmen)_2\{Ag(CN)_2\}_2][Zn(Dmen)_2(H_2O)_2]\{Ag(CN)_2\}_2$ (Dmen = *N*,*N'*-Dimethylethylenediamine)[1]

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Abstract—A cyanido bridged Zn(II)-Ag(I) bimetallic complex (**I**) has been prepared and characterized by IR spectroscopy, thermal analysis, X-ray crystallography (CIF file CCDC no. 884016) and DFT calculations. Thermal analysis shows that the composition of the compound is consistent with the proposed stoichiometry, i.e., $[Zn(diamine)_2\{Ag(CN)_2\}_2] \cdot H_2O$. The crystal structure of complex **I** consists of two independent molecules; a trinuclear molecule, $[Zn(Dmen)_2\{Ag(CN)_2\}_2]$ and an ionic species, $[Zn(Dmen)_2\text{-}(H_2O)_2]\{Ag(CN)_2\}_2$; the overall formula being $[Zn(Dmen)_2\{Ag(CN)_2\}_2][Zn(Dmen)_2(H_2O)_2]\{Ag(CN)_2\}_2$ (**I**) (Dmen = *N*,*N'*-dimethylethylenediamine). The structures of **I** and two of its analogues, $[Zn(Dmen)_2\{Ag(CN)_2\}_2]_2 \cdot 2H_2O$ (**II**) and $\{[Zn(Dmen)_2\{Ag(CN)_2\}][Ag(CN)_2]\}_2 \cdot 2H_2O$ (**III**) were predicted by DFT calculations. The DFT results reveal that the structure **I** is more stable in comparison to the calculated structures, **II** and **III**. The X-ray structure of **I** shows that the complex is also stabilized by the argentophilic interactions. The Ag···Ag interaction energy calculated at the MP2 level of theory is –4.02 kcal mol^{-1}.

Keywords: zinc(II), silver cyanide, *N*,*N'*-dimethylethylenediamine, DFT

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INTRODUCTION

Dicyanidoargentate(I), $[Ag(CN)_2]^-$ is a ligand of medium field strength [1]. It can coordinate either as a terminal [2, 3] or as a bridging ligand [4–15] and sometimes behaves only as a counter ion [16–18]. $[Ag(CN)_2]^-$ has been widely employed as a bridging unit for the preparation of coordination polymers [5–15]. The interplay between covalent and argentophilic (Ag–Ag) interactions generates numerous bimetallic M-Ag(I) compounds exhibiting a variety of structures comprising not only of $[Ag(CN)_2]^-$ [5–15, 19, 20] but also of the $[Ag_2(CN)_3]^-$ [21] and $[Ag_3(CN)_5]^{2-}$ units [22]. In addition, the compounds incorporating oligomeric units of $[Ag(CN)_2]^-$ such as trimeric, $\{[Ag(CN)_2]^-\}_3$ [3] and pentameric $\{[Ag(CN)_2]^-\}_5$ [23] units have also been isolated. In an attempt to examine the structural features of such complexes, we have previously reported the crystal structures of a number of $[Ag(CN)_2]^-$ containing bimetallic compounds [2–5, 17, 18]. In this work, we report the structural and theoretical analysis of another Zn(II)–Ag(I) bimetallic complex, $[Zn(Dmen)_2\{Ag(CN)_2\}_2]$-$[Zn(Dmen)_2(H_2O)_2]\{Ag(CN)_2\}_2$ (**I**) (Dmen = *N*,*N'*-dimethylethylenediamine). To better understand the role of $[Ag(CN)_2]^-$ ligands on the stability of complexes, the DFT optimized structures of two related complexes, $[Zn(Dmen)_2\{Ag(CN)_2\}_2] \cdot 2H_2O$ (**II**) and $\{[Zn(Dmen)_2\text{-}\{AgCN)_2\}][Ag(CN)_2]\}_2 \cdot 2H_2O$ (**III**) are also presented.

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[1] The article is published in the original.

EXPERIMENTAL

Materials and instrumentation. $ZnCl_2$ and Dmen were obtained from Merck Chemical Co., Germany. $AgNO_3$ was a product of Panreac, Spain. $K[Ag(CN)_2]$ was prepared by reacting $AgNO_3$ with KCN in a 1 : 2 mol ratio in water. The IR spectrum of the complex was recorded with a Perkin Elmer FTIR spectrophotometer in the 4000–500 cm^{-1} range. The solid state thermal gravimetric (TG) analysis of the title complex was carried out on TGA/SDAT 851 e Mettler Tolledo USA under argon atmosphere at the heating rate of 10°C min^{-1}.

Synthesis of I. To a solution of 1 mmol (0.136 g) $ZnCl_2$ in 10 mL in water were added 2 mmoles of Dmen in 15 mL methanol. After stirring for 15 min, 0.40 g (2 mmol) of $K[Ag(CN)_2]$ in 15 mL distilled water was added to the aforementioned solution. The reaction mixture was stirred for further 30 min at room temperature. After filtration, the residue was collected and dried in air. The crystals of **I** were obtained from the filtrate by keeping it in air for overnight.

X-ray crystallography. Data collection for **I** was performed at 173 K with a Stoe Mark II-Image Plate Diffraction System equipped with a two-circle goniometer and using MoK_α graphite monochromated radiation. The structure was solved by direct methods with SHELXS-97 [24, 25] and refined by full-matrix least squares procedures on F^2 using the program SHELXL-97 [24, 25]. All non-hydrogen atoms were refined anisotropically. All hydrogen atom positions, except of the N-bonded hydrogen atoms, were refined using a riding model. The positions of N-bonded hydrogen atoms were taken from the difference Fourier map and refined isotropically. The dimethylethylenediamine ligand was disordered and split into two parts. The crystals were of poor quality, therefore the refinement resulted in a somewhat high R value. The crystal data and details of the data collection are summarized in Table 1.

Crystallographic data for the structure **I** have been deposited with the Cambridge Crystallographic Data Center (CCDC no. 884016; deposit@ccdc.cam.ac.uk or www.ccdc.cam.ac.uk).

Theoretical (DFT) calculations. Theoretical studies were performed for **I** as well as for its two analogues **II** and **III**. In the case of complex **I**, for the initial geometry in the optimization procedures, the fragment of the crystallographic structure was used. The calculations were performed by using B3LYP-D3 method (standard hybrid density functional B3LYP [26, 27] method with dispersion correction D3 [28]) and combined basis sets LanL2DZ [29] for Ag and Zn atoms in conjunction with the D95V(d,p) [30] basis set for all other atoms. The calculations were performed for the complexes investigated in the gas phase as well as in water solvent by using the polarizable continuum model (PCM) [31, 32].

The atomic charges and second-order interaction energies were calculated with DFT method using the NBO program [33, 34]. All computations were carried out with Gaussian 09 set of programs [35].

RESULTS AND DISCUSSION

IR spectrum of **I** was studied in the range 4000–500 cm^{-1}. The vibrational frequencies and IR intensities have been computed for the model complex investigated in the gas phase as well as in water solution. The B3LYP-D3 calculated vibrational frequencies and IR intensities as well as the bands observed in the experimental infrared spectrum along with their assignments are collected in Table 2. The vibrational assignment of the experimental spectrum was performed by examination of the calculated atomic displacements and visualization of the normal modes of the model complex **I**.

As follows from Table 2, two strong and broad bands (the most intense ones) due to the N–H and O–H stretching mode were observed at 3261 and 3300 cm^{-1}, respectively. The calculated values of these modes are 3502 and 3526 cm^{-1} (in the gas phase) and 3390 and 3454 cm^{-1} (in water solvent), respectively. The presence of Dmen ligands is manifested by two bands of C–N stretching modes of diamine at 1070 and 1088 cm^{-1}. The calculated frequencies follow the experimentally observed values of these modes and appear at 1097 and 1122 cm^{-1} (in the gas phase) and 1096 and 1120 cm^{-1} (in solvent), respectively. The ν(C–N) stretching band also occurs at lower frequency (851 cm^{-1}) and is connected with bending mode of O–H group. This signal in DFT analysis appears at 863 and 852 cm^{-1} for gas and solvent, respectively. The other strong bands at 2152 and 2136 cm^{-1} indicate the C≡N stretching vibrations from bridged and terminal $[Ag(CN)_2]^-$ ligands [3, 9, 36]. With respect to the bridged C≡N ligands these vibrations are overestimated in theoretical spectrum by about 100 cm^{-1}. The strong peak at 952 cm^{-1} was assigned to N–H bending vibration and is in good accordance with the theoretical results.

The thermal behavior of the synthesized complex **I** was studied by TG analysis to detect the different decomposition processes and to confirm the proposed stoichiometry. The results of thermal analysis given in Table 3 indicate a good correlation between the calculated and found weight loss values for the investigated complex. The thermal decomposition pattern of expected **I** is depicted in Fig. 1. The decomposition starts at about 110°C and is completed at 570°C. At the first stage water is released between 110–190°C corresponding to the weight loss of 3.5% (calcd. 3.1%). The second weight loss (31.7%, calcd. 30.4%) relates to the elimination of two Dmen molecules. The removal of Dmen takes place in two steps. The removal of one

Table 1. Crystallographic data and refinement details for compound **I**

Parameter	Value
Formula	$C_{12}H_{12}N_8OZnAg_2$
Formula weight	565.41
Crystal system	Triclinic
Space group	$P\bar{1}$
a, Å	7.0003(8)
b, Å	8.9093(9)
c, Å	17.1286(19)
α, deg	85.470(9)
β, deg	82.500(9)
γ, deg	74.755(8)
V, Å^3	1020.71(19)
Z	2
ρ_{calcd}, g cm^{-3}	1.840
μ(MoK_α), mm^{-1}	3.079
F(000)	544
Crystal size, mm	0.50 × 0.45 × 0.20
Temperature, K	173(2)
λ(MoK_α), Å	0.71073
2θ Range, deg	1.19–26.22
Index ranges h, k, l	$-8 \le h \le 8$, $-10 \le k \le 10$, $-20 \le l \le 21$
Max. and min. transmission	0.749 and 0.315
Reflections collected/unique (R_{int})	12307/3856 (0.0894)
Reflections observed ($I > 2\sigma(I)$)	3253
Data/restraints/parameters	3856/0/23
R_1, wR_2, S ($I > 2\sigma(I)$)	0.0980, 0.2660, 1.058
Largest diff. peak and hole, e Å^{-3}	5.629 and −1.410

Dmen molecule takes place at 265°C and that of the other at 460°C. The next weight loss of 11% occurs between 470–570°C due to the removal of 2CN$^-$ (calcd. 8.98%). Thus, the proposed formula of the complex is $[Zn_2(Dmen)_4(H_2O)_2\{Ag(CN)_2\}_4]$. This composition agrees with the formula determined by crystallographic studies (vide infra).

The molecular structure of complex **I** and the crystallographic numbering scheme are illustrated in Fig. 2. The selected bond length and bond angle are given in Table 4. The crystal structure of the complex consists of two independent molecules; a centrosymmetric trinuclear molecule with the formula $[Zn(Dmen)_2\{Ag(CN)_2\}_2]$ and an ionic species, $[Zn(Dmen)_2(H_2O)_2]\{Ag(CN)_2\}_2$, the overall formula being $[Zn(Dmen)_2\{Ag(CN)_2\}_2Zn(Dmen)_2(H_2O)_2\{Ag(CN)_2\}_2]$. This formula fits exactly to the results of TG studies. The trinuclear molecule is made up of two $[Ag(CN)_2]^-$ anions linked to a $[Zn(Dmen)_2]^{2+}$ unit through CN$^-$ in a *trans* configuration. The Zn^{2+} ions, which are located on centers of inversion, assume slightly distorted octahedral geometry with four nitrogen atoms of the diamines and two CN$^-$ nitrogen atoms completing the coordination sphere. One of the CN$^-$ is attached to silver(I) through nitrogen. The coordination environment of the $[Ag(CN)_2]^-$ units is close to linear (angle CAgN 176.0(4)°). The shortest Ag(1)–Ag(2) distance between two trinuclear units is 3.2987(14) Å, which is just below the threshold of argentophilic interactions [3, 20]. In the cationic complex of the ionic species, zinc is coordinated by two Dmen and two water molecules adopting a distorted octahedral geometry. The water molecules are attached to zinc in a *trans* configuration. The coordination environment of the $[Ag(CN)_2]^-$ counter ion is nearly linear (angle CAgC 179.1(6)°).

The theoretical (DFT) calculations were performed for the complex **I** and two of its analogues **II**

Table 2. Experimental IR data for **I** and DFT calculated frequencies (cm^{-1}) and intensities (km mol^{-1}) for the model complex (intensities are given in brackets)

Experiment*	Gas	Water	Assignment
3300 s	3390 (740)	3454 (1128)	ν(OH)
3261 s	3502 (277)	3526 (444)	ν(NH)
2928 s	3034 (63)	3053 (191)	$\nu_{sym}(CH_3)$
2152 m	2247 (210)	2253 (164)	ν(CN)
2136 m	2137 (205)	2147 (104)	ν(CN)
1471 m	1487 (20)	1481 (21)	δ(CH)
1435 m	1452 (14)	1450 (19)	δ(CH) + δ(NH)
1351 w	1387 (13)	1387 (20)	δ(CH)
1286 w	1304 (18)	1307 (22)	δ(CH)
1143 m	1162 (35)	1169 (80)	δ(CH)
1088 m	1122 (50)	1120 (72)	$\nu(CN)_{Dmen}$
1070 m	1097 (24)	1096 (59)	$\nu(CN)_{Dmen}$
1034 m	1049 (32)	1050 (69)	δ(CH)
1005 m	1019 (55)	1018 (72)	δ(CH)
952 s	962 (189)	969 (419)	δ(NH)
851 s	863 (61)	852 (230)	$\delta(OH) + \nu(CN)_{Dmen}$
711 s	723 (11)	788 (344)	δ(OH)

* ν = stretching; δ = bending; m = medium; s = strong; w = weak.

Table 3. TG data of the zinc(II) complex $Zn_2(Dmen)_4(H_2O)_2\{Ag(CN)_2\}_4$

Decomposition range, °C	Weight loss, %		Group removed	DSC peak temperature, °C*
	found	calculated		
110–190	3.1	3.5	H_2O	180.8 (endo)
265–460	31.7	30.4	Dmen	353.8 (endo)
470–570	11.0	9.0	CN^-	428.7 (exo)

* exo means exothermic and endo means endothermic.

and **III** in the gas phase as well in water solvent by using PCM [32, 33]. These two approaches allow us to compare the results obtained for the system in different conditions. In the gas phase the crystal packing effects and strong H-bonding interactions are omitted, while in the solvent (water) the conditions are closer to that in the crystal. In the optimization procedures the fragment of the crystallographic structure was taken as the starting geometry. Figure 3 presents the fully optimized structure of complex **I**, investigated in water solvent. The structures of the complexes **II** and **III** optimized at the BLYP-D3 level in water are illustrated in Fig. 4.

The selected geometric parameters (bond distances and angles between atoms) of complex **I** calculated at the DFT level of theory are collected in Table 4. According to the obtained results, the calculated bond distances in most cases are overestimated with respect to the X-ray determined values. To compare the reproducibility of the experimental interatomic distances and the bond angles in two applied approaches (in the gas phase and in the solvent), the corresponding values of the root mean square deviations (RMSD's) have been calculated as shown in Table 4. With respect to these results, better agreement between the theoretical and experimental bond distances was obtained for the calculations performed for the complexes investigated in the solvent (RMSD is 0.194 Å). The same conclusions can be drawn for the bond angles (RMSD 5°).

Table 5 collects the relative values of electronic energies (ΔE_e), enthalpies (ΔH) and Gibbs free energies (ΔG) of the studied complexes. According to these results, the complex **I** is the most stable one. The val-

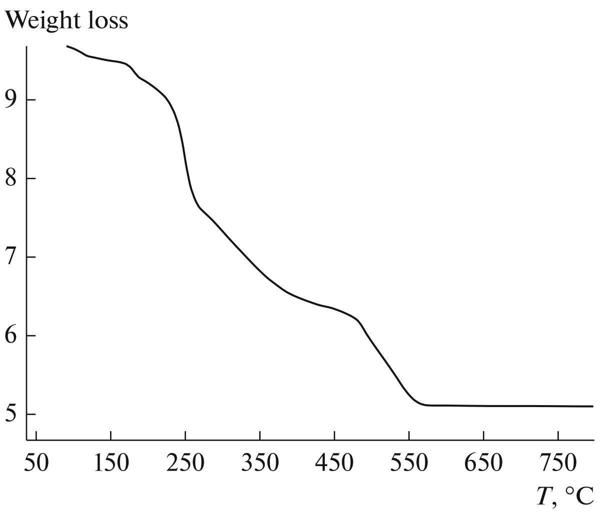

Fig. 1. TGA curve of complex **I**.

ues of ΔG (in water solvent) are smaller than those calculated for complexes **II** and **III** by 16.44 and 18.02 kcal mol^{-1}, respectively. The results obtained for the complexes investigated in the gas phase revealed that the complex **II** is less stable than **III** by 11.76 kcal mol^{-1}.

The X-ray structure of **I** shows that it is also stabilized by the argentophilic interactions. The shortest distance between Ag atoms of two trinuclear units (Ag(1)···Ag(2)) is 3.2987(14) Å, which is smaller than the sum of the van der Waals radii of the Ag atoms (3.44 Å) [20]. The theoretical investigation of the model dimers of H–Ag–PH$_3$ and Cl–Ag–PH$_3$ are performed in [37]. The calculated equilibrium Ag···Ag distances for those complexes are 2.845 and 2.866 Å, respectively. The MP2 interaction energies (ΔE) calculated for the H–Ag–PH$_3$ and Cl–Ag–PH$_3$ dimers are equal to –7.92 and –9.30 kcal mol^{-1}, respectively. They also calculated ΔE at the self-consistent field (SCF) level. The corresponding values are 4.47 and 4.68 kcal mol^{-1}.

With respect to the complex investigated in the current work the question arises, how strong the Ag···Ag interaction is? To answer this question the model complex based on the fragment of the crystal structure of **I** was built (Fig. 5). The hydrogen atoms were added to make the system neutral.

For the model complex the interaction energy was calculated by using SCF (HF) and MP2 methods.

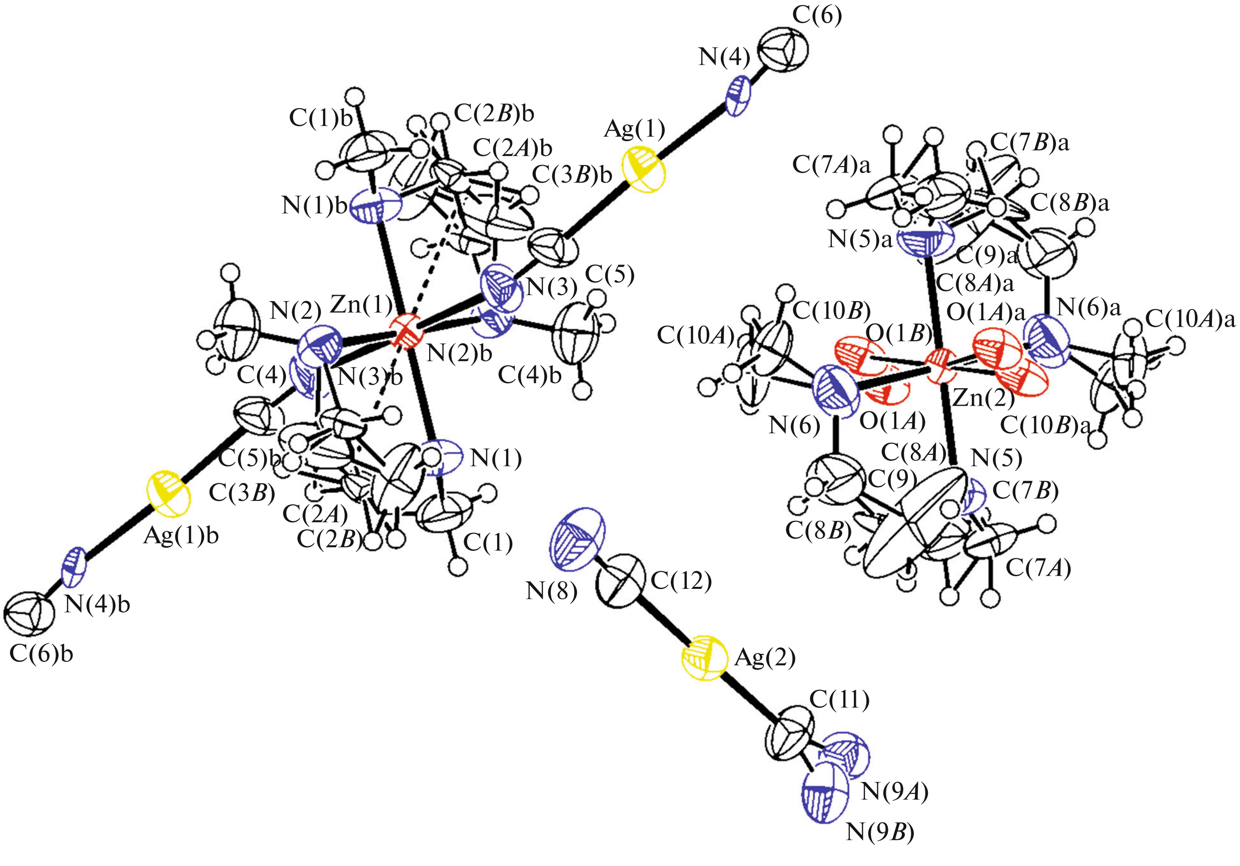

Fig. 2. Molecular structure of **I** showing the atom-numbering scheme.

Table 4. Selected bond lengths (d, Å) and angles (ω, deg) in complex **I**. Theoretical values calculated at the DFT (B3LYP-D3) level

Parameter	Experiment	Theory gas*	Theory water*
Bond	d, Å		
Ag(1)–C(5)	2.043(12)	2.061	2.070
Ag(1)–N(4)	2.078(8)	2.083	2.083
Zn(1)–N(1)	2.162(9)	2.252	2.228
Zn(1)–N(2)	2.155(10)	2.249	2.229
Zn(1)–N(3)	2.251(10)	2.162	2.198
Zn(2)–N(5)	2.141(11)	2.242	2.209
Zn(2)–N(6)	2.151(12)	2.247	2.220
Zn(2)–O(1*A*)	2.26(2)	2.257	2.229
Zn(2)–O(1*B*)	2.18(2)	2.160	2.213
Ag(2)–C(11)	2.047(14)	2.071	2.089
Ag(2)–C(12)	2.063(15)	2.082	2.097
Ag(1)–Ag(2)	3.2987(14)	4.519	4.001
N(1)–C(1)	1.414(18)	1.476	1.476
N(3)–C(5)	1.143(16)	1.170	1.171
RMSD**		0.332	0.194
Angle	ω, deg		
N(1)Zn(1)N(2)	85.4(4)	84.9	82.0
N(1)Zn(1)N(2)b	94.6(4)	97.4	98.2
N(1)bZn(1)N(2)b	85.4(4)	82.9	82.8
N(1)Zn(1)N(1)b	180.0(2)	178.9	178.0
N(1)Zn(1)N(3)	92.1(4)	93.0	93.3
N(1)bZn(1)N(3)	87.9(4)	85.9	88.4
N(2)Zn(1)N(3)	90.9(4)	88.6	92.0
N(2)Zn(1)N(3)b	89.1(4)	84.6	87.0
N(2)Zn(1)N(2)b	180.0(2)	175.5	179.4
N(3)Zn(1)N(3)b	180.0(4)	173.0	176.0
C(5)Ag(1)C(6)	176.0(4)	163.0	165.3
C(6)N(4)Ag(1)	165.8(9)	166.7	163.9
N(3)C(5)Ag(1)	175.6(11)	167.9	169.3
N(5)Zn(2)N(6)	83.0(5)	82.1	82.1
N(5)Zn(2)N(6)a	97.0(5)	100.5	103.2
N(5)Zn(2)N(5)a	180.0(1)	173.3	174.9
N(6)Zn(2)N(6)a	180.0(18)	176.7	174.6
N(5)Zn(2)O(1*A*)	88.0(7)	88.6	85.3
N(5)Zn(2)O(1*A*)a	100.9(7)	88.7	88.7
N(6)Zn(2)O(1*A*)	98.7(7)	98.4	93.2
N(6)aZn(2)O(1*A*)	88.2(7)	83.6	86.9
C(11)Ag(2)C(12)	179.1(6)	168.9	171.6
N(8)C(12)Ag(2)	178.4(14)	172.6	174.5
RMSD**		5.6	5.0

* Theoretical values calculated at the DFT (B3LYP-D3) level.

** Root mean square deviation.

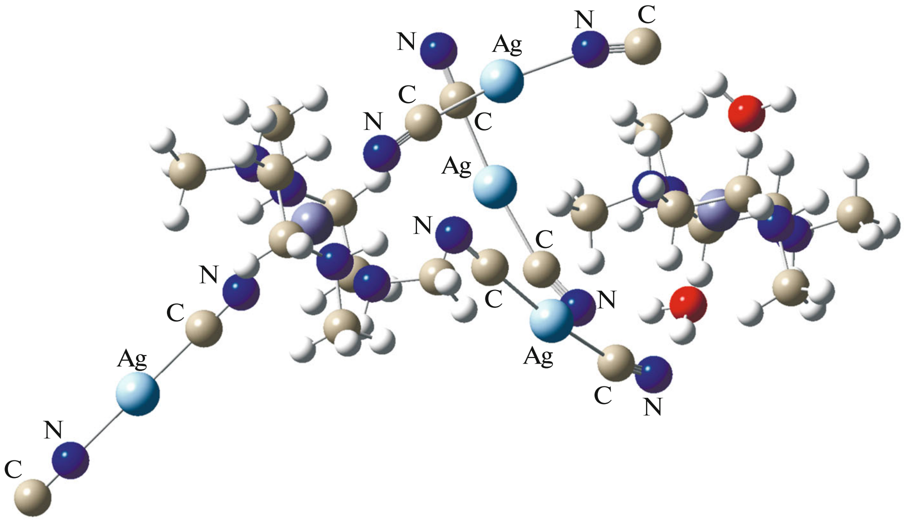

Fig. 3. Fully optimized structure of complex **I** (in water solvent).

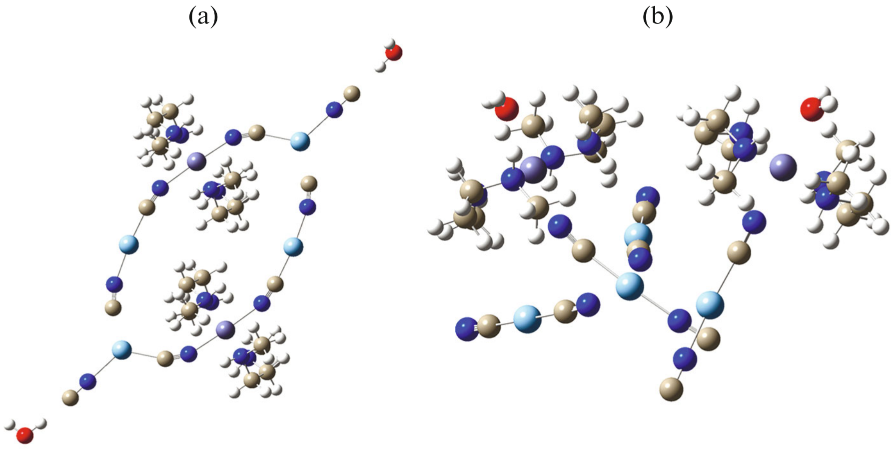

Fig. 4. Fully optimized structures of complexes **II** (a) and **III** (b) in water solvent.

Table 5. Relative values of electronic energies (ΔE_e), enthalpies (ΔH) and Gibbs free energies (ΔG) of complexes **I**, **II**, and **III** calculated at the B3LYP-D3/D95V(d,p)/LanL2DZ level of theory

Complex	In the gas phase			In water solvent		
	ΔE_{electr}	ΔH	ΔG	ΔE_{electr}	ΔH	ΔG
	kcal mol^{-1}					
I	0.00	0.00	0.00	0.00	0.00	0.00
II	31.55	30.88	25.03	29.15	27.61	16.44
III	11.62	11.48	13.27	25.09	24.89	18.02

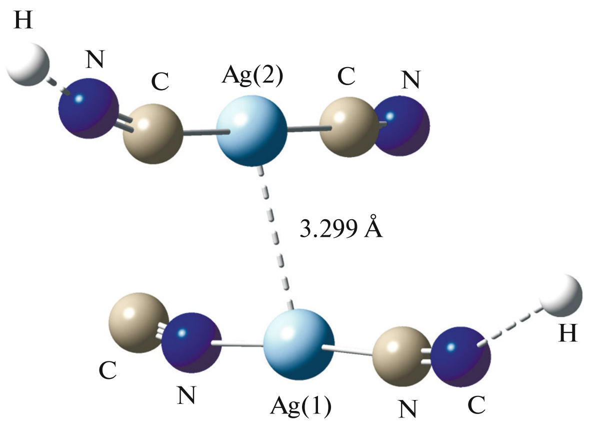

Fig. 5. Fragment of the crystal structure of **I** serving as a model in the calculations of the argentophilic interaction.

The SCF calculated Δ*E* is positive and equals 4.06 kcal mol^{-1}. This value is similar to that obtained for the H–Ag–PH_3 and Cl–Ag–PH_3 dimers [37]. Therefore, according to the SCF method the model complex is unstable. The MP2 calculated interaction energy is negative (–4.02 kcal mol^{-1}), which indicates that the model complex is stable. The difference between the values of Δ*E* calculated at the SCF and MP2 levels of theory reveals the significant role of electron correlation effects (mainly dispersion energy) in stabilization interaction of the model complex.

The NBO charges on selected atoms of model complex are reported in Table 6. According to these data, the charges on the Ag(1) and Ag(2) atoms are different. The value of the charge on Ag(1) is 0.547 e (in the gas phase) while on the Ag(2) atom the charge is smaller by 0.145 e. This can be explained as a consequence of the different surroundings. The Ag(1) atom is directly bound to the C and N atoms while Ag(2) is bonded to two carbon atoms. The similar situation has been found with respect to the zinc(II) cations. The charges on Zn(1) and Zn(2) are 1.309 and 0.138 e, respectively. As follows from the obtained results, the absolute values of the charges on the N atoms of the Dmen ligand (N(1), N(1)b, N(2), N(2)b) range from –0.822 to –0.792 e in the gas phase and –0.812 to 0.798 e in water. They are larger than those found on the N atoms of CN^- bridged ligands (N(3) and N(4)).

The NBO analysis also revealed a few very weak second-order interactions between orbitals of the Ag atoms. The strongest one (0.79 kcal mol^{-1}) corresponds to a donation of the electron density from the lone pair (LP) orbital on Ag(1) to the antibonding Rydberg orbital (RY*) on Ag(2). Figure 6 illustrates orbitals involved in this LP(Ag(1)) → RY*(Ag(2)) interaction.

In conclusion, the present study describes that the structure of $[Zn(Dmen)_2\{Ag(CN)_2\}_2][Zn(Dmen)_2(H_2O)_2]\{Ag(CN)_2\}_2$ (**I**) is a combination of a neutral molecule and an ionic species. In both components, zinc atom displays octahedral geometry. The DFT calculations reveal that the experimental structure **I** is more stable in comparison to the two model complexes, $[Zn(Dmen)_2\{Ag(CN)_2\}_2]_2 \cdot 2H_2O$ (**II**) and $\{[Zn(Dmen)_2\{Ag(CN)_2\}][Ag(CN)_2]\}_2 \cdot 2H_2O$ (**III**). The structure of **I** is stabilized by the argentophilic interactions. The Ag···Ag interaction energy calculated at the MP2 level of theory is –4.02 kcal mol^{-1}.

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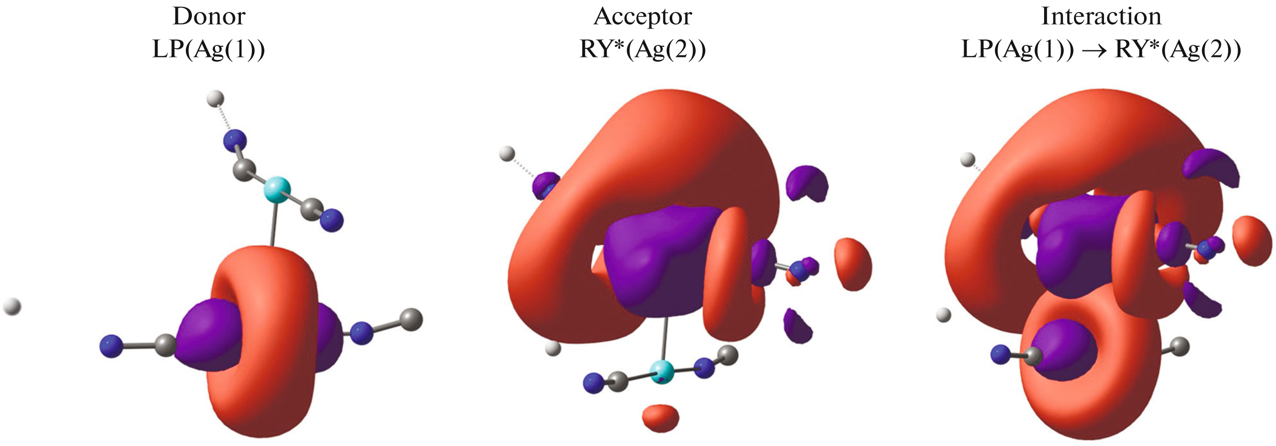
Donor
LP(Ag(1))

Acceptor
RY*(Ag(2))

Interaction
LP(Ag(1)) → RY*(Ag(2))

Fig. 6. The donor and acceptor orbitals involved in the strongest LP(Ag(1)) → RY*(Ag(2)) interaction.

Table 6. NBO charges on selected atoms of complex **I**

Atom	*q*, e (in gas)	*q*, e (in water)
Ag(1)	0.547	0.559
N(1)	–0.794	–0.800
N(1)b	–0.796	–0.803
N(2)	–0.792	–0.798
N(2)b	–0.822	–0.812
N(3)	–0.686	–0.673
N(4)	–0.718	–0.749
C(5)	0.056	0.032
Zn(1)	1.309	1.311
Zn(2)	1.447	1.452
O(1*A*)	–1.050	–1.044
O(1*A*)a	–1.081	–1.056
Ag(2)	0.402	0.443
C(11)	–0.009	–0.034
C(12)	–0.060	–0.074

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