Egypt. J. Chem. **58**, No. 1, pp. 71- 83 (2015)

Equilibrium Studies of Complex Formation Reactions of $[Pd(SMC)(H_2O)_2]^+$ with Amino Acids, Peptides or DNA Constituents

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COMPLEX-FORMATION equilibria have been investigated for $[Pd(SMC)(H_2O)_2]^+$ where SMC = *S*-methyl-L-cysteinate, with amino acids, peptides and DNA constituents. Stoichiometries and stability constants of the complexes were determined at 37°C and constant ionic strength (0.16 M $NaNO_3$). The results showed the formation of 1:1 complexes with amino acids .Peptides formed both 1:1 complexes and the corresponding deprotonated amide species. DNA constituents formed both 1:1 and 1:2 complexes .The binding mode of the ligands containing various functional groups was studied and the speciation diagrams were evaluated.

Sulfur-containing biomolecules such as cysteine (Cys), methionine (Met), glutathione (GSH), metallothionein (MT) and albumin play significant roles in platinum anticancer chemotherapy because of their high affinity to platinum (II) compounds [1-5]. The bidentate N, S-complex was found to be promising cytostatic agent [6]. Sulfur is involved in the entire metabolic process of platinum drugs, including reactions prior to cell uptake, deactivation prior to DNA binding and formation of DNA-adduct, … etc [7]. On the other hand, the platinum sulfur interactions can be used to produce favorable effects in the clinical application of Pt-based drugs. It is possible now to employ sulfur-containing compounds as chemoprotectants to mitigate the severe toxic side effects of platinum drugs and some of them have been registered in a number of European countries [8-10]. Furthermore, Methionine, cysteine, and pencillamine are believed to be determinant in the reduction of the nephrotoxicity of cis-platin and other chemotherapeutic drugs[11]. A previous investigation [12] focused on the kinetics of the interaction of diaqua-(*S*-methyl-L-cysteinate) palladium(II) with some DNA constituents. It seemed of interest to extend this work to throw more light on the speciation of Pd(*S*-methyl-L-cysteinate) complexes, as a model for the main metabolite in cancer chemotherapy, in biological fluids where all types of ligands are present. Furthermore, the results of this study are of interest because it is possible to make some comparisons with the chemistry of metabolites of Pt(II) anticancer complexes. The present investigation describes the formation equilibria involving $[Pd(SMC)(H_2O)_2]^+$ (SMC = *S*-methyl-L-cysteinate) and

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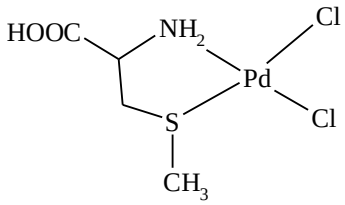
other ligands such as amino acids, peptides or DNA constituents at 37°C and constant ionic strength (0.16 M $NaNO_3$).

Experimental

Materials

K_2PdCl_4, and *S*-methyl-L-cysteinate were obtained from Aldrich. The amino acids and related compounds (glycine, alanine, valine, proline, ethanolamine, serine, threonine, histidine, histamine, ornithine, lysine, cysteine, methionine) were provided by Sigma Chemical Co. The peptides used (glycinamide, glycylglycine, glycylleucine, glutamine) were all provided by BDH Biochemicals Ltd., Poole, England. The DNA constituents (Inosine, Inosine-5-monophosphate, uracil, thymine , uridine and uridine-5-monophosphate) were provided by Sigma Chemical Co. The complex $[Pd(H\text{-}SMC)Cl_2].H_2O$, where H-SMC is *S*-methyl-L-cysteinate, was prepared as described before.[12] (Anal. Found: C, 14.60; H, 3.36; N, 4.27. Calc.: C, 14.52; H, 3.32; N, 4.24 %.) The complex was converted in solution into the diaqua form by treating it with two equivalents of $AgNO_3$, as described elsewhere [13–15] .



$[Pd(SMC)Cl_2]$

Potentiometric measurements

Potentiometric measurements were performed using a Metrohm 751 Titroprocessor. The electrode and titroprocessor were calibrated with standard buffer solutions prepared according to NBS specifications [16]. All titrations were carried out at 37 ± 0.1 ◦ C and 0.16 M ionic strength (adjusted with NaNO3) in purified nitrogen atmosphere using a titration vessel described previously[17]. The ligands were converted into their protonated form with standard HNO_3 solutions. The acid dissociation constants of the ligands were determined by titrating 1.25 mmol samples of each with standard 0.05 M NaOH solutions. The acid dissociation constants of the coordinated water molecules in $[Pd(H\text{-}SMC)(H_2O)_2]^{2+}$were determined by titrating 1.25 mmol of the complex with standard 0.05 M NaOH solution. The formation constants of the complexes were determined by titrating solution mixtures of $[Pd(H\text{-}SMC)(H_2O)_2]^{2+}$ (1.25 mmol) and the ligand in the concentration ratio of 1:1 for amino acids and peptides and in the ratio of 1 : 2 (Pd : ligand) for the DNA constituents. The titrated solution mixtures , each had a volume of 40 ml.

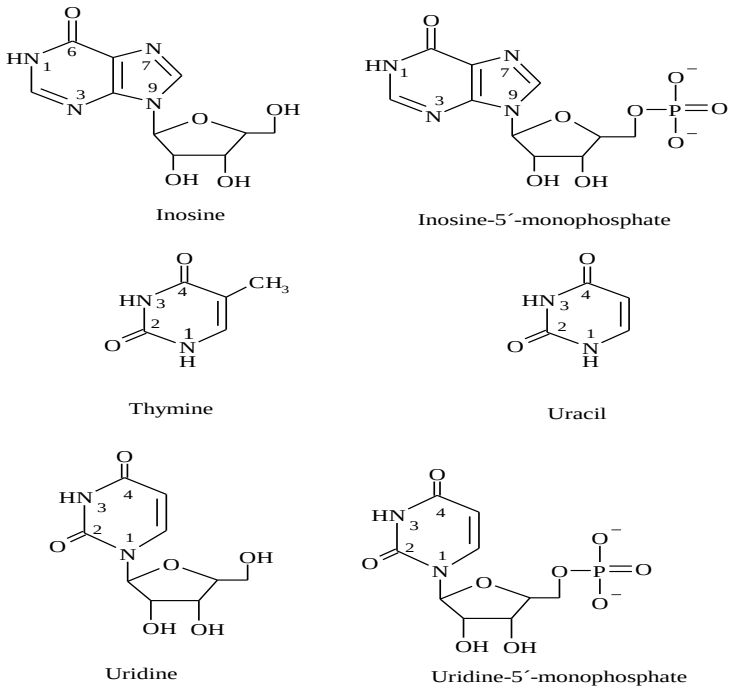
The species formed were characterized by the general equilibrium process (1), whereas the formation constants for these generalized species are given by Eq. (2) (charges are omitted for simplicity).

$$pM + qL + rH \rightleftharpoons M_p L_q H_r \quad (1)$$

$$\beta_{pqr} = \frac{[M_p L_q H_r]}{[M]^p [L]^q [H]^r} \quad (2)$$

where the charges are omitted for simplicity.

M, L and H represent [Pd (SMC)$(H_2O)_2]^+$, ligand and proton, respectively. The calculations were performed using the program MINIQUAD-75 [17] running on an IBM-486 computer. Stoichiometric and stability constants of the complexes were determined by trying various possible composition models for the systems studied. The selected model gave the best statistical fit and was chemically consistent with the titration data without giving any systematic drift in the magnitude of various residuals, as described elsewhere [17]. The stability constants of the complexes formed in solution are given in Table 1. The concentration distribution diagrams were obtained with the program SPECIES [18], taking into account the experimental conditions used.



Scheme1. Structural formula of some of the investigated ligands.

TABLE 1. Formation constants for complexes of binary complexes involving pd(ii).

System	M	L	H [a]	log β [b]	pK$_a$ [c]
Pd(SMC)-OH	1	0	-1	-3.81(0.03)	3.81
	1	0	-2	-14.37(0.03)	10.56
	2	0	-1	-0.58(0.05)	3.23
Glycine	0	1	1	9.20(0.02)	9.20
	0	1	2	11.02(0.03)	1.82
	1	1	0	9.71(0.02)	
Alanine	0	1	1	9.27(0.01)	9.27
	0	1	2	11.17(0.02)	1.90
	1	1	0	9.83(0.01)	
Valine	0	1	1	9.01(0.01)	9.01
	0	1	2	10.98(0.02)	1.97
	1	1	0	9.65(0.03)	
S-methyl-L-cysteinate	0	1	1	8.49(0.02)	8.49
	0	1	2	10.42(0.03)	1.93
	1	1	0	8.76(0.04)	
Proline	0	1	1	10.06(0.01)	10.06
	0	1	2	11.81(0.05)	1.86
	1	1	0	10.11(0.03)	
Ethanolamine	0	1	1	9.16(0.01)	9.16
	1	1	0	7.34(0.02)	
	1	2	0	11.82(0.04)	
	1	1	-1	0.50(0.02)	6.84
Serine	0	1	1	8.59(0.01)	8.59
	0	1	2	10.95(0.02)	2.36
	1	1	0	9.36(0.07)	
	1	1	-1	0.24(0.08)	9.12
Theronine	0	1	1	8.79(0.01)	8.79
	0	1	2	10.85(0.02)	2.06
	1	1	0	9.22(0.02)	
	1	1	-1	0.04(0.05)	9.18
Histidine	0	1	1	8.84(0.01)	8.84
	0	1	2	14.74(0.02)	5.90
	0	1	3	16.81(0.06)	2.07
	1	1	0	11.28(0.04)	
Histamine	0	1	1	9.34(0.01)	9.34
	0	1	2	15.20(0.02)	5.86
	1	1	0	10.63(0.09)	
Ornithine	0	1	1	9.81(0.02)	9.81
	0	1	2	18.16(0.02)	8.35
	1	1	0	10.12(0.01)	
	1	1	1	18.89(0.01)	8.77
Lysine	0	1	1	9.91(0.02)	9.91
	0	1	2	18.80(0.03)	8.89
	1	1	0	10.02(0.02)	
	1	1	1	18.86(0.03)	8.84
Cysteine	0	1	1	10.00(0.01)	10.00
	0	1	2	18.21(0.01)	8.21
	0	1	3	19.62(0.01)	1.41
	1	1	0	13.11(0.05)	
	1	1	1	21.75(0.03)	8.64
Methionine	0	1	1	8.76(0.02)	8.76
	0	1	2	10.98(0.03)	2.12
	1	1	0	8.43(0.04)	

TABLE .1 Contd.

System	M	L	H[a]	log β[b]	pK[ac]
Glycinamide	0	1	1	7.50(0.02)	7.50
	1	1	0	7.13(0.02)	
	1	1	-1	3.38(0.02)	3.56
Glycylglycine	0	1	1	7.50(0.02)	7.50
	1	1	0	7.13(0.02)	
	1	1	-1	3.38(0.02)	3.56
Glycylleucine	0	1	1	7.91(0.01)	7.97
	0	1	2	10.92(0.01)	2.95
	1	1	0	7.19(0.02)	
	1	1	-1	1.96(0.06)	5.23
Glutamine	0	1	1	8.77(0.01)	8.37
	0	1	2	10.78(0.02)	2.01
	1	1	0	8.14(0.05)	
	1	1	-1	1.00(0.05)	7.14
Inosine	0	1	1	8.43(0.03)	8.43
	1	1	0	6.15(0.03)	
	1	2	0	9.86(0.02)	
Inosine-5´-monophosphate	0	1	1	8.83(0.02)	8.83
	0	1	2	14.94(0.03)	6.11
	1	1	0	7.18(0.01)	
	1	2	0	11.61(0.02)	
Uracil	0	1	1	8.98(0.01)	8.98
	1	1	0	7.48(0.04)	
	1	2	0	11.92(0.05)	
Thymine	0	1	1	9.35(0.01)	9.35
	1	1	0	8.23(0.06)	
	1	2	0	13.01(0.01)	
Uridine	0	1	1	8.77(0.01)	8.77
	1	1	0	7.22(0.03)	
	1	2	0	11.31(0.03)	
Uridine-5´-monophosphate	0	1	1	9.23(0.01)	9.23
	0	1	2	15.12(0.02)	5.99
	1	1	0	8.17(0.03)	
	1	2	0	12.92(0.04)	

[a]M, L and H are the stoichiometric coefficients corresponding to Pd(SMC),amino acids, peptides or DNA units, and H^+ respectively; Standard deviations are given in parentheses and sum of square of residuals are less than $5e^{-7}$.

Results and Discussion

Hydrolysis of $[Pd(SMC)(H_2O)_2]^+$

The $[Pd(SMC)(H_2O)_2]^+$ion may undergo hydrolysis. Its acid–base chemistry was characterized by fitting the potentiometric data to various acid–base models. The best-fit model was found to be consistent with the formation of three species: 10-1, 10-2 and 20-1, as given in reactions (3)–(5). The equilibrium

constants were determined at temperature 37 °C and at constant 0.16 M ionic strength (adjusted with $NaNO_3$), and given in Table 1. These values were taken into account on determining the stability constants of the Pd^{II} complexes.

$$[Pd(SMC)(H_2O)_2]^+ \overset{pK_{a1}}{\rightleftharpoons} [Pd(SMC)(H_2O)(OH)] + H^+ \quad (3)$$

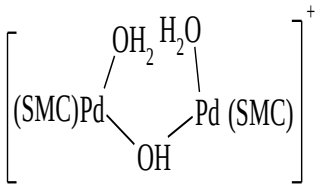
100 10-1

$$[Pd(SMC)(H_2O)(OH)] \overset{pK_{a2}}{\rightleftharpoons} [Pd(SMC)(OH)_2]^- + H^+ \quad (4)$$

10-1 10-2

$$[Pd(SMC)(H_2O)_2]^+ + [Pd(SMC)(H_2O)(OH)] \overset{\log K_{dimer}}{\rightleftharpoons}$$

100 10-1



$$+ H_2O \quad (5)$$

20-1

The μ-hydroxo species (20−1) is assumed to form through dimerization of the Pd(II) complex via a hydroxo group. The equilibrium constant for the dimerization reaction (5) can be calculated by Eq. (6) and amounts to 3.23.

$$\log K_{dimer} = \log\beta_{20-1} - \log\beta_{10-1} = -0.58 - (-3.81) = 3.23 \quad (6)$$

The concentration distribution diagram for $[Pd(SMC)(H_2O)_2]^+$ complex is shown in Fig. 1. The concentration of the monohydroxo species, 10-1 and the dimeric species, 20-1, increase with increasing pH. The dimeric species has maximum concentration of 40% at pH ~ 3.8. The monohydroxo species (10-1) is the main species in the pH range ~ 4.0-10.6, *i.e.* it is the main species present under physiological conditions. A further increase in pH is accompanied by an increase in the dihydroxo species (10-2), which is the main species above pH *ca.*10.6.

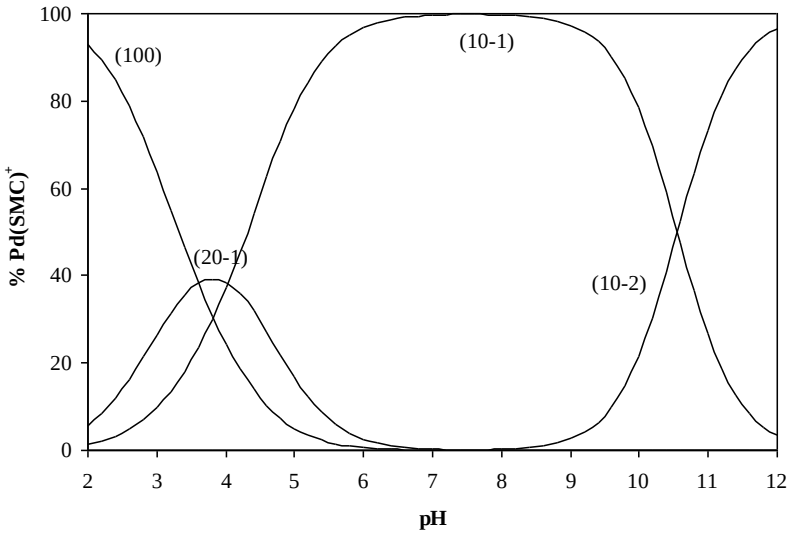


Fig.1. Concentration distribution of various species as a function of pH in the Pd(SMC)-OH system at concentration of 1.25 mmole/liter for Pd(SMC).

Complex-formation equilibria involving amino acids

Analysis of the titration data for the Pd(SMC)-amino acid system showed the formation of 1:1 species. The stability constant of the histidine and ornithine complexes are higher than those of simple amino acids. This indicates that these amino acids coordinate via the two nitrogen centers, *i.e.* imidazole and amino groups in the case of histidine, and by two amino groups in the case of ornithine. This is in line with the strong affinity of Pd^{II} for nitrogen donor centers. The stability constant of the complex with lysine (log β_{110} =10.02) is a little bit higher than those of α-amino acids. This may be taken to indicate that lysine most likely chelates through the α -amino and carboxylate groups (N, O-donor set). The proline complex has the highest value. This may be due to the highest basicity of the proline amino group as reflected by the highest pKa value. The stability constant value of methionine complex (log β_{110} = 8.43) is lower than those of most simple amino acids. This may be explained by the fact that the amino group of methionine is less basic than those of other amino acids as reflected by pK_a values, (Table 1). *S*-methyl-L-cysteinate forms a more stable complex than methionine although the pK_a of the former is lower than the latter. This may be accounted for on the premise that the five-membered chelate ring in the former complex is energetically more stable than the six-membered chelate ring in the latter complex. Serine and threonine have an extra binding center on the β-alcoholate group. This group was reported [19] to participate in transition metal ion complex-formation reactions. the potentiometric data is much better fitted assuming the formation of the complex species 110 and 11–1. The pK_a value of the β- alcoholate group incorporated in the Pd^{II} complex, (logβ_{110} –log β_{11-1}) is

9.12 and 9.18 for serine and threonine, respectively. In addition, ethanolamine forms the complex species 110, 120 and 11–1, and the $\log\beta_{110}$ value for ethanolamine is smaller than those for amino acids. This may be due to the coordination of ethanolamine at low pH through the amino group, while in the case of serine and threonine the coordination is through amino and carboxylate groups. The p*K*a value of the coordinated alcohol group in ethanolamine (6.84) is smaller than those of serine and threonine. This is attributed to the tendency of ethanolamine to coordinate through the OH group at lower pH to form a five member chelate ring. The cysteine complex is significantly more stable than those of the amino acids (N,O-donor site) and ornithine (N,N donor site). This indicates that cysteine coordinates via S- and N-donor sites. This is consistent with the high affinity of both S and N atoms for coordination to the Pd(II) ion.

The concentration distribution diagram (Fig. 2) indicates that serine forms the species 110 at low pH and predominates between pH ~2.7-9.2 and thus prevents the hydrolysis of Pd (II), *i.e*. the species (10-1) and (20-1) are present at very low concentration. The ionisation of the OH group starts after pH ~7 and the (11-1) species predominate after pH ~ 9.2.

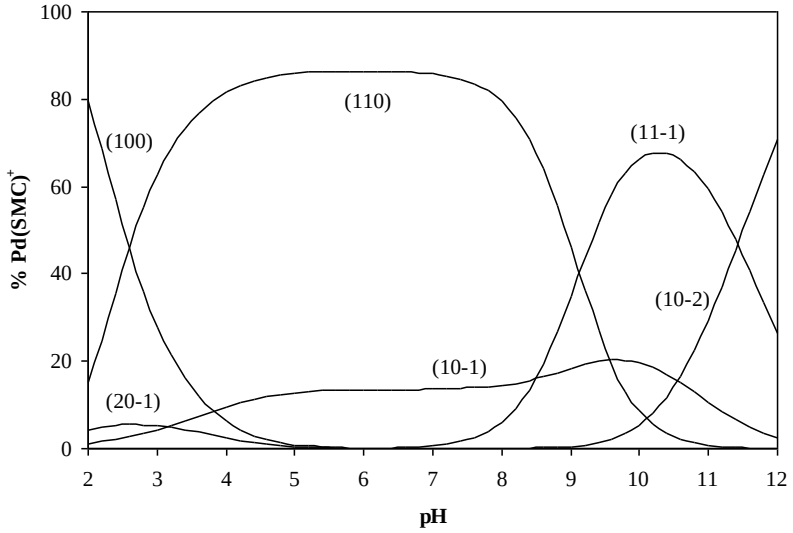
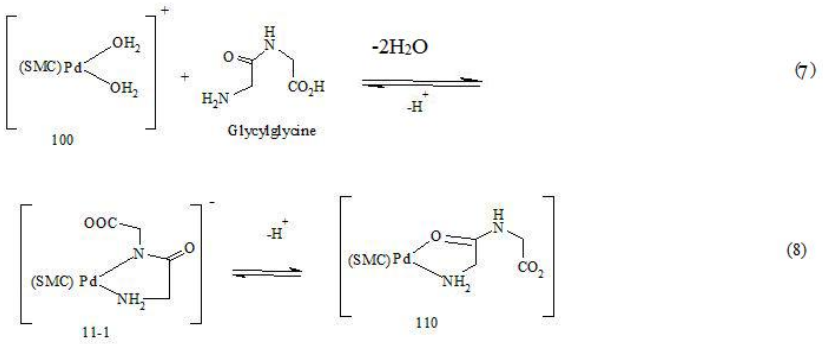


Fig. 2. Concentration distribution of various species as a function of pH in the Pd(SMC) and Serine system. (at concentration of 1.25 mmole/liter for Pd(SMC) and Serine).

Complex-formation equilibria involving peptide

The complex formation equilibria involving peptides were characterized by fitting their potentiometric data to various models. The best model was found to be consistent with the formation of the complexes with stoichiometric

coefficients 110 and 11-1 according to Eq. (7) and (8) (see Table 1).The complexes are formed by coordination of the amino and carbonyl groups. Upon deprotonation of the amide group, the coordination sites would switch from carbonyl oxygen to amide nitrogen. Such changes in coordination centers are well documented [20]. The glutamine complex is more stable than the glycinamide complex. The most likely explanation lies in the fact that glutaminate carries a negative charge, whereas glycinamide is neutral. The electrostatic interaction between the glutaminate and the twofold positively charged metal complex would result in a lowering of free energy of formation. The pKa values of the amide groups, incorporated in the palladium(II) complexes (logβ110 - logβ11-1) are in the range of 3.56-7.14. The low pKa values in the present system are probably due to the high affinity of palladium to nitrogen-type ligands. It is interesting to note that the pKa value for the glycinamide complex is lower than those for other peptides. This can be explained on the premise that the more bulky substituent group on the peptide may hinder the structural changes when going from the protonated to the deprotonated complexes. The pKa of the glutamine complex is exceptionally higher than those of the other peptide complexes. This is due to the formation of a seven membered chelate ring which is more strained and therefore less favoured.



Scheme 2. The Complex-formation equilibria for peptides.

The relative magnitudes of the pKa values of the palladium(II) complexes with peptides have interesting biological implications. Under normal physiological conditions (pH ca. 7.4), the peptides would coordinate with $[Pd(SMC)(H_2O)_2]^+$ in entirely different fashions: glutaminate exists solely in its protonated form, whereas the other peptides are present entirely in the deprotonated form. Also, the slight differences in the side chains of the peptides seem to produce dramatic differences in their behavior towards the palladium species.

The concentration distribution diagram (Fig. 3) indicates that glycylglycine forms the complex species (110) at low pH and (11-1) at higher pH. The species

(11-1) is the main species at higher pH and predominantes after pH 4.6 for glycylglycine.

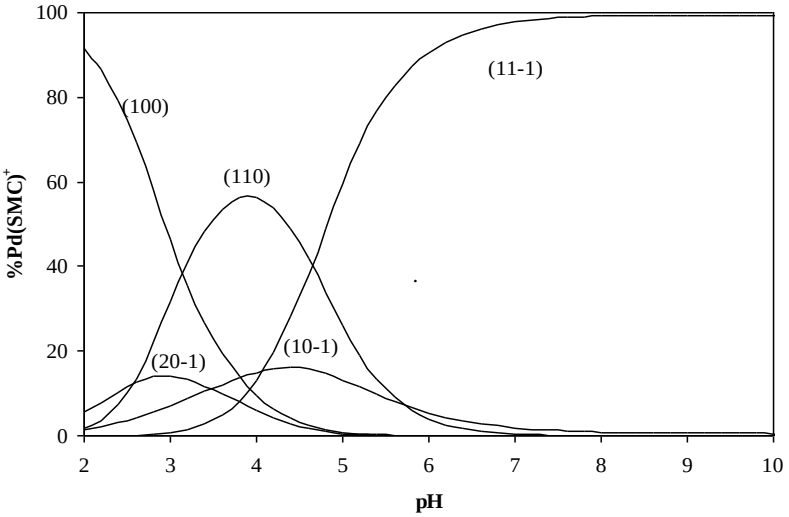


Fig. 3. Concentration distribution of various species as a function of pH in the Pd(SMC)-glycylglycine system. (at concentration of 1.25 mmole/liter for Pd(SMC) and glycylglycine).

Complex-formation equilibria involving DNA constituents

DNA constituents such as Inosine, Inosine -5′-monophosphate, uracil, thymine,Uridine-5′-monphosphate , and uridine form 1 : 1 and 1 : 2 complexes with$[Pd(SMC)]^+$. Inosine can be protonated at N7 forming a (N1H-N7H) monocation. The pK_a of N1H is 8.43, Table 1. The pK_a of N7H is 1.2. [21] It was reported [21] that, in the acidic pH range, N1 remained protonated, while the metal ion is coordinated to N7. The binding site at the higher pH was disputed and it was suggested that there is a gradual change from N7- binding to N1-binding with increase of pH. [21]. Inosine-5´-monophosphate (5´-IMP) forms a more stable complex with $[Pd(SMC)(H_2O)_2]^+$ than that of inosine. The extra stabilization can be attributed to the triply negatively charged 5´-IMP^{3-} ion. N_3 is the preferred complexation site of the 4-oxo-pyrimidine derivatives as uracil, thymine, uridine and uridine-5´-monophosphate. The pK_a values of N_3H given in Table 1, are consistent with the literature values[22, 23]. The stability constants of the 4-oxo-pyrimidine derivatives are larger than most of DNA constituents due to their high basicity. The thymine complex is more stable than that of uracil, probably due to the higher basicity of the N3 site of thymine resulting from the inductive effect of the extra electron-donating methyl.

The concentration distribution diagrams for Pd(SMC)-inosine, complex, (Fig. 4) show that the species 20-1, 10-1, 10-2, are the predominated species (above pH=3). This means that the complex formation of $[Pd(SMC)(H_2O)_2]^+$ with

inosine does not prevent hydrolysis. For Pd(SMC)- inosine the species 110 reaches a maximum concentration of (7.3%) at pH ~ 6.4. The species 120 reaches a maximum concentration of (15.2%) at pH ~ 8.4. The species 10-1 and 20-1 compete with 110 and 120 species. The dihydroxy species prevails after pH ~ 10.6.

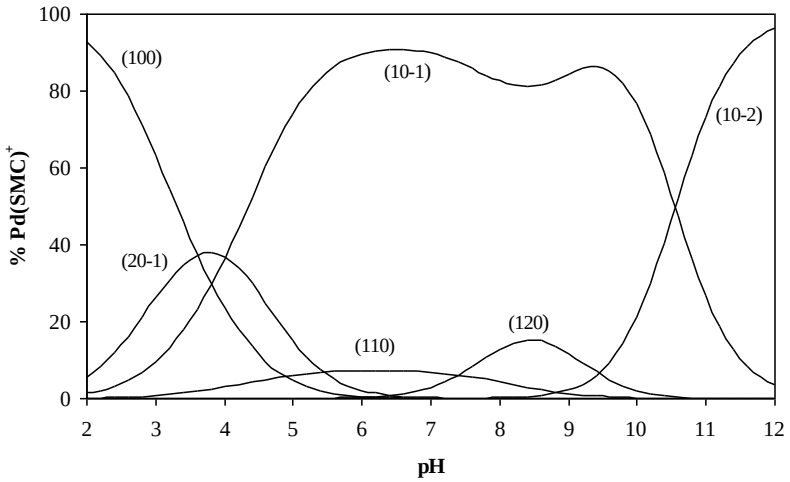


Fig. 4. Concentration distribution of various species as a function of pH in the Pd(SMC)-Inosine system. (at concentration of 1.25 and 2.50 mmole/liter for Pd(SMC) and Inosine, respectively).

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(Received 18 / 1 / 2015,
accepted 28 / 1 / 2015)

دراسة اتزان تكوين المتركبات الناتجة من تفاعل المتراكب الثنائى$^+$[Pd (SMC)$(H_2O)_2$]مع الاحماض الامينية،البيبتيدات او مكونات DNA

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تم فى هذا البحث دراسة اتزان تكوين المتركبات الناتجة من تفاعل المتراكب $^+$[$Pd(SMC)(H_2O)_2$] (حيث ان SMC = كبريت مثيل سستين) مع الاحماض الامينية ، البيبتيدات او مكونات DNA، وتم التعرف على النسب الجزيئية لهذه المتراكبات ، وكذلك تم حساب ثوابت الاستقرار لها عند درجة حرارة 37^{o}م وقوة ايونية 0.16 مولارى من نترات الصوديوم . اتضح من النتائج تكوين متراكبات بالنسبة الجزئية 1:1 مع الاحماض الامينية وتكون البيبتيدات متراكبات بالنسبة الجزئية 1:1 بالاضافة الى متراكبات منزوعة البروتون من مجموعة الاميد وتكوين متراكبات بالنسب الجزئية 1:1 و 1:2 مع وحدات DNA كما تم شرح طريقة الارتباط للمرفقات المحتوية على المجموعات الوظيفية المختلفة وحساب تركيز المتراكبات المتكونة فى المحلول كدالة فى رقم الاس الهيدروجينى للوسط.