

Theoretical Studies for Arsenic Interferences by Inductively Coupled Plasma Mass Spectrometer

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A study on the thermochemistry of species ($^{40}\text{Ar}^{35}\text{Cl}^+$, $^{59}\text{Co}^{16}\text{O}^+$, $^{36}\text{Ar}^{38}\text{Ar}^1\text{H}^+$, $^{38}\text{Ar}^{37}\text{Cl}^+$, $^{36}\text{Ar}^{39}\text{K}^+$, $^{150}\text{Nd}^{++}$, $^{150}\text{Sm}^{++}$ and $^{150}\text{Eu}^{++}$) that interfere with arsenic in inductively coupled plasma mass spectrometer was estimated by Gaussian code. Moreover, (AsCH_3F^+ , AsF^+ , AsCH_2^+ , AsCHF^+ and AsO^+) that result from the reactions between arsenic and different gases such as H_2 , O_2 and CH_3F , which are commonly used in dynamic reaction cell-inductively coupled plasma- mass spectrometer, have been investigated. The structures of polyatomic molecules are optimized; ionization energies, heats of formation ($\Delta_f H^\circ_0$ and $\Delta_f H^\circ_{298}$) and proton affinity (PA) of some species are estimated by theoretical calculations using different methods in Gaussian.

Keywords: Arsenic interferences/ Gaussian 09 / DRC-ICP-MS

Introduction

Arsenic (As) which has a single isotope in 100% abundance is one of the most toxic elements in nature. Exposure to arsenic causes irritation in stomach and intestines for humans and it also causes decreased production of red and white blood cells, skin damages and lung irritation. The exposure to Arsenic can also cause infertility and cancer, may lead to life loss [1]. Determination of arsenic in water, soils, and biological samples requires sensitive analytical techniques. Atomic absorption [2], fluorescence detection [3] and inductively coupled plasma mass spectrometer (ICP-MS) [4,5] are the usual techniques for determination of arsenic. ICP-MS is the most preferable technique for arsenic determination especially in case of very low concentrations. However, this technique suffers from polyatomic

interfering species which are formed due to the effect of plasma temperature and need high resolution for separation [6]. Interfering ions could be observed with argon containing ions such as $^{40}\text{Ar}^{35}\text{Cl}^+$, $^{36}\text{Ar}^{38}\text{Ar}^1\text{H}^+$, $^{38}\text{Ar}^{37}\text{Cl}^+$, $^{23}\text{Na}^{12}\text{C}^{40}\text{Ar}^+$ and $^{40}\text{Ar}^{34}\text{SH}^+$ and, other polyatomic ions like $^{59}\text{Co}^{16}\text{O}^+$, $^{43}\text{Ca}^{16}\text{O}_2^+$, $^{12}\text{C}^{31}\text{P}^{16}\text{O}_2^+$ and $^{40}\text{Ca}^{35}\text{Cl}^+$ (Table 1).

Arsenic is a mono-isotope of mass 75, therefore when interferences occur it is not possible to switch to an alternative isotope. Theoretical studies about the combination of these species in the plasma condition is important and helps for improving the ability of the instrument by decreasing the possibility of polyatomic interfering species combination. Good instrumental conditions

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during the measurement process are very important and may decrease the interferences effect and can also improve the precision and the detection limits especially at low concentrations. The spectral interferences can be separated using high resolution mass spectrometers [8]. The problem of high resolution mode, is decreasing the intensity of the signal which makes the instrument less sensitive especially for low concentrations [9]. Moreover, the high resolution ICP-MS does not cover all needed resolutions. Therefore, inductively coupled plasma mass spectrometer with collision/reaction cell^[4,6] have been developed and used for eliminating the spectral interferences in quadrupole ICP-MS. Collision/Reaction Cells (CRCs) have been developed to work in two modes, one of them is the reaction mode, in which, a reactive gas like (CH₃F, H₂, N₂O, O₂, N₂, Cl₂) is

used to remove the reactive interferences from the analyte isotope. The other mode is the collision mode which uses a non-reactive gas like helium gas, and the cell in this case doesn't operate under thermal conditions or chemical reactions. In this process, the polyatomic interferences can be removed or discriminated because of kinetic energy discrimination (KED) in which all polyatomic ions are larger than the analyte ions having the same mass. Hence, the analyte atomic ions, which have the highest kinetic energy pass through the cell, and the interfering polyatomic ions having lower kinetic energy do not pass through the cell, resulting in polyatomic interference reduction. These low energy ions are removed from the ion beam by the effect of bias voltage at the cell exit [10,11].

Table (1): polyatomic ions of Mass 75 and the required resolution needed for separation[7].

Interfere molecule	Mass	\Delta m	Required resolution	Interfere molecule	Mass	\Delta m	Required resolution
⁴⁰ Ar ³⁵ Cl ⁺	74.9312	0.0096	7770	⁴³ Ca ¹⁶ O ₂ ⁺	74.9486	0.0270	2775
⁵⁹ Co ¹⁶ O ⁺	74.9281	0.0065	11495	²³ Na ¹² C ⁴⁰ Ar ⁺	74.9522	0.0306	2452
³⁶ Ar ³⁸ Ar ¹ H ⁺	74.9381	0.0165	4538	¹² C ³¹ P ¹⁶ O ₂ ⁺	74.9636	0.0420	1784
³⁸ Ar ³⁷ Cl ⁺	74.9286	0.0070	10641	⁴⁰ Ar ³⁴ SH ⁺	74.9381	0.0165	4546
³⁶ Ar ³⁹ K ⁺	74.9313	0.0097	7757	⁴⁰ Ca ³⁵ Cl ⁺	74.9314	0.0098	7607

The target of our work is to discuss the interferences of As and these different reactions in the collision cell. Target gases such as hydrogen in mixture with helium gas[8,9] have been used to remove the Ar₂⁺ interfering ions^[4,6], the interference of ⁴⁰Ar³⁵Cl with As can be decreased through the reaction: 2⁴⁰Ar³⁵Cl⁺ + H₂ → 2⁴⁰Ar⁺ + 2HCl[12]. Arsenic ion signal can shift to AsO⁺ by oxidizing agents such as O₂ through the reaction M⁺ + ½ O₂ → MO⁺ [13] or N₂O[9,14,15] through the reaction M⁺ + N₂O → MO⁺ + N₂. As also can be shifted to AsCH₂⁺ by using CH₃F as a reaction gas through the reaction M⁺ + CH₃F → MCH₂⁺ + HF[16]. There are different species that can be combined during this reaction in the reaction cell, like MCH₃F⁺, MF⁺, MCH₂⁺, MCHF⁺, CH₂F⁺. Eduardo et. al [17] used CH₃F as a reactant gas and found that ⁷⁵As¹²CH₂⁺ is the respective favored reaction product ions during the measuring process which shift the m/z for arsenic from 75 to 89. The mechanisms that may be involved inside the reaction/collision cell are: charge exchange or

proton, hydride ion, or atom (H, O, etc.) transfers, depending upon the element cation and the reaction gas[18,19]. Arsenic also interferes with (¹⁵⁰Nd⁺⁺, ¹⁵⁰Sm⁺⁺) (m/z = 75). In this case, a theoretical correction must be done by switching to another isotope for each of them which free from any interference. Therefore, in this study, quantum chemistry composite methods (G3, CBS-Q, MP2/CEP-4G and MP3/CEP-4G) are used for performing the ionization energy and heats of formation of the species of interest at 0K and 298K in gas phase.

Experimental considerations:

Polyatomic ions of ⁴⁰Ar³⁵Cl⁺ interferences which result from the presence of chlorine can be decreased experimentally in the instruments which have no collision cell. In the present case, Joel plasma high resolution ICP-MS is used at a low resolution mode to optimize the RF power to decreasing the effect of chlorine in dilute HCl

solution, and this is clear in (fig. 1), which shows the ratio $^{40}\text{Ar}^{35}\text{Cl}^+ / ^{35}\text{Cl}^+$ to get the optimum RF value for measuring As^+ signal with the small value of interferences. It is clear that the RF value according to (fig. 1) is 1100 Watt.

The calculated ratio $^{40}\text{Ar}^{35}\text{Cl}^+ / ^{35}\text{Cl}^+$ is 0.0103, and this small value is obtained by decreasing the RF value, and this may be due to that the ionization energies of (As^+ , ArCl^+ , Cl^+ and Ar^+ are 9.46,

11.72, 11.78 and 14.66 eV respectively, as shown in Table (3). The obtained ratio can be used to correct the interference which results from the presence of chlorine according to the equation: $\text{As} = \text{As}^* - 0.0103 \times ^{35}\text{Cl}^+$, where As refers to the corrected value, As^* refers to the measured value which interfere with $^{40}\text{Ar}^{35}\text{Cl}^+$ and $^{35}\text{Cl}^+$ is the measured chlorine in the sample which causes the interference problem.

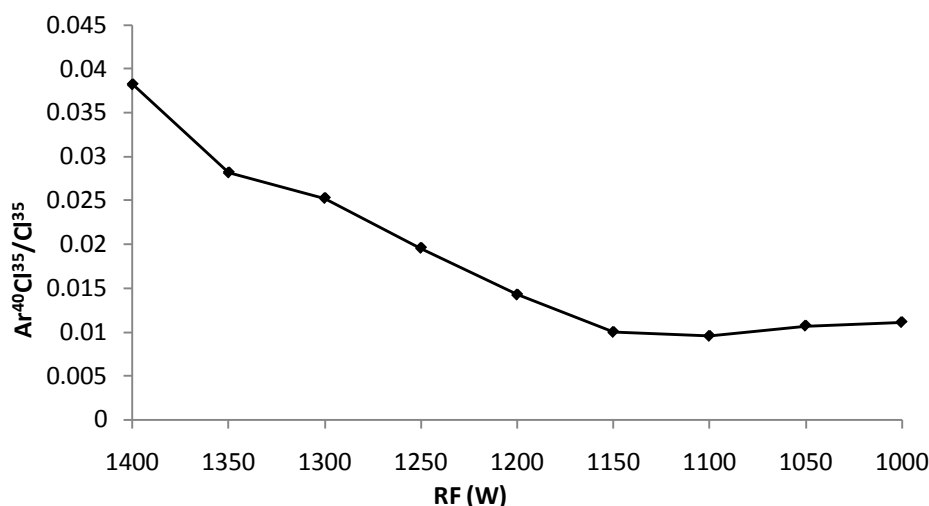


Fig. (1) : the relation of $^{40}\text{Ar}^{35}\text{Cl}^+ / ^{35}\text{Cl}^+$ as a function of RF Power

Theoretical Considerations:

The levels of theory used in this work include the four composite methods (G3, CBS-Q, MP2/CEP-4G and MP3/CEP-4G) in Gaussian code of programs [20]. These methods of calculation work according to different theories[21,22] such, Gaussian-3 (G3) theory which is the third in a series of Gx methods for calculation of molecular energies. In this method a sequence of well-defined ab initio molecular orbital calculations is performed to arrive at a total energy of a given molecular species. Geometries are determined using second-order Moller-Plesset (MP2) perturbation theory. Correlation level calculations are done using Moller-Plesset perturbation theory up to fourth-order and with quadratic configuration interaction. (CBS) means complete basis set and energy calculation run with this method is computationally cheap and has high accuracy. CBS methods approximate an infinitely large basis set by combining energies from many lower-level

theories. The MP-energy corrections are obtained from Rayleigh-Schrodinger (RS) perturbation theory with the unperturbed Hamiltonian which is defined as:

$$\hat{H}_0 = \hat{F} + \langle \Phi_o | \hat{H} - \hat{F} | \Phi_o \rangle \quad (1)$$

and the perturbation defined as the correlation potential

$$\hat{V} = \hat{H} - \hat{H}_0 = \hat{H} - (\hat{F} + \langle \Phi_o | \hat{H} - \hat{F} | \Phi_o \rangle) \quad (2)$$

Where the normalized Slater determined (Φ_o) is the lowest eigenstate of the fock operator

$$\hat{F}\Phi_o = \sum_{K=1}^N \hat{F}(K)\Phi_o = 2 \sum_{i=1}^{N/2} \varepsilon_i \Phi_o \quad (3)$$

Where N is the number of electrons in the molecule, \hat{H} is the usual electronic Hamiltonian, $\hat{F}(K)$ is the one –electron fock operator and ε_i is the orbital energy.

MP₂ formula for a closed-shell molecule is given as:

$$E_{MP2} = \frac{1}{4} \sum_{i,j,a,b}^N \frac{\langle \Phi_i \Phi_j | \hat{V} | \Phi_a \Phi_b \rangle \langle \Phi_a \Phi_b | \hat{V} | \Phi_i \Phi_j \rangle}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b} \quad (4)$$

Where Φ_i and Φ_j are canonical occupied orbitals, Φ_a and Φ_b are virtual (or unoccupied)

orbitals. The quantities $\varepsilon_i, \varepsilon_j, \varepsilon_a$ and ε_b are the corresponding orbital energies.

In MP₃ perturbation theory, the energy is given as:

$$E_{MP3} = \sum_{Sr}^D \frac{\hat{V}_{OS} (\hat{V}_{Sr} - \hat{V}_{00} \delta_{Sr}) \hat{V}_{t_0}}{(E_0 - E_s)(E_0 - E_t)} \quad (5)$$

Where the summation is held over the set of all doubly excited determinants D, and the O index indicates $\psi_n^{(0)}$, the zero-order wave functions.

Results and Discussion

Heats of formation, at 0 K ($\Delta_f H^\circ_0$), is obtained theoretically from the computed atomization energies of the individual species combined with the experimental gas phase 0 K heats of formation of the constituent atoms[23] and temperature correction to enthalpy ($H^\circ_{298} - H^\circ_0$), are obtained using the theoretical correction calculated for the species of interest and the experimental contribution for the constituent elements[24]. Thermochemical data, which used in the calculations, are shown in Table (2).

$\Delta_f H^\circ_0$ and $\Delta_f H^\circ_{298}$ are calculated by applying methods G3 and CBS-Q, which have good precision on the calculation of thermochemical quantities such as heats of formation, $\Delta_f H^\circ_{298}$, adiabatic ionization energies, IE, and proton affinities, PA. The selected species are optimized to obtain its geometry structure which has the lowest energy for each structure and used to calculate harmonic frequencies.

Adiabatic ionization energies (IE) for each atom or molecule which result from the effect of plasma temperature are obtained by calculating the difference in total atomization energies at 0 K of the cation and the corresponding neutral atom at their respective optimized geometries. Tables (3), shows the calculated adiabatic ionization energies, IE for the cations under study and the species

The expected reaction between the analyte (A^+) and gas (G) gives $A + G^+$ due to charge exchange and this can occur if the ionization energy of the reacted gas is less than the ionization energy of the analyte i.e. $IE(G) < IE(A)$. The same reactant can also give $(A-H) + GH^+$ by the effect of Proton transfer and this process is known as proton affinity (PA), which can happen only if $PA(G) > PA(A-H)$.

Table (2): $\Delta_f H^\circ_0$ for the constituent atoms and ($H^\circ_{298} - H^\circ_0$) for the constituent elements in (kJ/mol).

Constituent atoms	$\Delta_f H^\circ_0$ (kJ/mol)	Constituent elements	($\Delta_f H^\circ_{298} - \Delta_f H^\circ_0$) kJ/mol
Ar	0.0	Ar (g)	6.197
H	216.035	H ₂ (g)	8.468
Cl	119.6	Cl ₂ (g)	9.181
O	249.18	O ₂ (g)	8.68
N	472.68	N ₂ (g)	8.67
K	89	K (s)	7.088
Ca	177.8	Ca (s)	5.736
Na	107.5	Na (s)	6.46
C	716.68	C (s)	1.05
P	316.5	P (s)	5.36
S	277.17	S (s)	4.412
As	303	As (s)	6.2
Sm	207	Sm (s)	7.6
Nd	328	Nd (s)	7.2
Eu	175	Eu (s)	8

which can interfere with As during the measuring process using ICP-MS.

The IE calculations in Table (3) may help to understand the probability of interfering ions during the analysis process using ICP-MS This is because it enables to predict whether the reaction between the analyte ion A^+ and the reactant gas G can occur or not. It can occur only if $IE(G) < IE(A)$, as clear from the data in Table(3) and this can be happened by the same manner for proton affinity, $PA(X)$, according to the reaction ($XH^+ \rightarrow X + H^+$). It can be calculated for X as follows: $PA(X) = H^\circ_{298}(X) - H^\circ_{298}(XH^+) + 6.2$ kJ/mol, where the latter term is the enthalpy of the proton at 298 K. Proton affinity of $^{36}\text{Ar}^{38}\text{ArH}^+$ and $^{40}\text{Ar}^{34}\text{SH}^+$ are calculated using the G3 and CBS-Q methods of calculations and their calculated values are 326.112 and 866.742, respectively. The heats

of formation of the selected species are shown in Table(4), where H°_0 refers to the sum of electronic and zero-point energies and H°_{298} refers to the sum of electronic and thermal enthalpies. The species ($^{40}\text{Ar}^{35}\text{Cl}^+$, $^{36}\text{Ar}^{38}\text{ArH}^+$, $^{38}\text{Ar}^{37}\text{Cl}^+$, $^{36}\text{Ar}^{39}\text{K}^+$, $^{150}\text{Nd}^{++}$, $^{150}\text{Sm}^{++}$ and $^{150}\text{Eu}^{++}$) can interfere with As. This interference depends on the matrix of the samples itself. For (^{150}Nd , ^{150}Sm) these isotopes are stable isotopes and with abundances 5.64 and 7.4, respectively. (^{150}Eu is radioactive isotope with half life 36 y).

Table: (5) shows reactions of arsenic with different gasses in the dynamic reaction cell in ICP-MS. In case of using CH_3F in the dynamic reaction cell, there are four possible cases of interactions

between CH_3F and arsenic ($\text{As}^+ + \text{CH}_3\text{F}$). The species which result from these reactions are (AsCH_3F^+ , AsF^+ , AsCH_2^+ , AsCHF^+) which can be measured experimentally^[17]. These different reactions can be explained as follows: First of them, the molecular addition which give (AsCH_3F^+). This reaction is exothermic ($\Delta_f H^{\circ}_{298} = -200.19$ KJ/mol). This reaction can also give ($\text{AsF}^+ + \text{CH}_3$) in case of transferring of fluorine atom to give AsF^+ , and this reaction is endothermic ($\Delta_f H^{\circ}_{298} = 58.82$ KJ/mol). By elimination of HF from CH_3F , the reaction gives $\text{AsCH}_2^+ + \text{HF}$ ($\Delta_f H^{\circ}_{298} = -31.27$ KJ/mol). Also because of the dehydrogenation of CH_3F , the products $\text{AsCHF}^+ + \text{H}_2$ ($\Delta_f H^{\circ}_{298} = 28.89$ KJ/mol) can be obtained.

Table (3): The ionization energies of elements (eV), which cause As interferences

Species	IE(eV)		Species	IE(eV)		
	G3	CBS-Q		G3	CBS-Q	Exp. ^[25,26]
CH_3F^+	11.80	11.79	As^+	9.46	9.48	9.789
AsCH_2^+	8.04	8.02	Ar^+	14.66	14.66	15.760
HF^+	13.89	13.95	Cl^+	11.78	11.78	12.968
AsO^+	8.01	8.12	Ca^+	5.12	5.12	6.113
O_2^+	12.41	12.33	O^+	12.01	12.03	13.618
Cl_2^+	11.19	11.19	H^+	13.56	13.56	13.598
ArCl^+	11.72	11.72	K^+	4.01	4.01	4.341
AsH^{++}	15.47	15.46	Na^+	4.96	4.96	5.140
H_2^+	14.61	14.61	P^+	9.94	9.94	10.487
AsCH_3F^+	8.12	8.21	C^+	10.72	10.73	11.260
AsF^+	9.14	9.29	F^+	15.59	15.64	17.423
AsCHF^+	7.82	7.91	N^+	13.97	13.97	14.534
CH_3^+	9.01	9.00	N_2^+	15.71	15.73	
CH_2F^+	8.45	8.46	S^+	9.15	9.15	10.360
ArAr^+	14.19	14.19	Ca^+	5.12	5.12	6.113
ArArH^+	10.23	10.23	CaO_2^+	13.04	14.66	
HCl^+	11.58	11.58				
ArSH^+	9.13	9.13				
CaCl^+	5.85	6.08		<i>MP2/CEP-4G</i>	<i>MP3/CEP-4G</i>	
ArSH^+	9.38	9.38	Nd^+	3.57	4.76	5.525
AsO^+	8.01	8.12	Nd^{++}	14.07	16.51	
ArK^+	3.97	3.97	Sm^+	3.89	3.44	5.644
NaCAr^+	5.74	6.03	Sm^{++}	20.17	17.77	
CPO_2^+	9.44	9.41	Eu^+	8.19	9.62	5.67
N_2O^+	11.06	11.08	Eu^{++}	17.15	18.80	

Table (4): Heat of formations of the species related to As interferences (kJ mol^{-1})

Species	G3		cbsq		Species	G3		cbsq	
	$\Delta_f H^\circ_0$	$\Delta_f H^\circ_{298}$	$\Delta_f H^\circ_0$	$\Delta_f H^\circ_{298}$		$\Delta_f H^\circ_0$	$\Delta_f H^\circ_{298}$	$\Delta_f H^\circ_0$	$\Delta_f H^\circ_{298}$
CH3F⁺	1403.18	1432.12	1408.57	1437.53	ArCl⁺	1389.68	1388.43	1389.68	1388.43
AsCH₂⁺	1507.71	1532.97	1484.23	1509.59	AsO⁺	1266.20	1284.37	1277.43	1295.61
HF⁺	1297.12	1314.45	1316.02	1333.34	ArCl⁺	1252.56	1274.09	1252.56	1274.09
AsCH₃F⁺	1295.54	1332.93	1290.26	1327.76	AsH⁺	6920.35	6940.02	1848.01	1867.68
AsF⁺	6129.88	6148.23	1096.95	1115.32	CoO⁺	1574.95	1575.54	924.42	925.60
AsCHF⁺	1399.54	1426.04	1391.73	1418.18	MP2/CEP-4G		MP3/CEP-4G		
CH₃⁺	1314.58	1338.28	1314.77	1338.47		$\Delta_f H^\circ_0$	$\Delta_f H^\circ_{298}$	$\Delta_f H^\circ_0$	$\Delta_f H^\circ_{298}$
CH₂F⁺	1173.76	1197.66	1182.17	1206.08	Nd⁺	328	341.3962	328	341.3988
HCl⁺	1176.61	1194.11	1176.61	1194.11	Nd⁺	671.9799	685.3761	787.7408	801.137
ArS⁺	1399.85	1399.21	1399.85	1399.21	Nd⁺	1685.68	1699.076	1920.704	1934.103
ArAr⁺	1368.72	1366.16	1368.72	1366.16	Sm⁺	207	220.7962	207	220.7988
CaO₂⁺	1143.98	1144.06	1834.30	1836.52	Sm⁺	582.0369	595.8331	539.1809	552.9797
NaCAr⁺	1264.65	1266.75	1293.41	1296.50	Sm⁺	2152.758	2166.554	1921.16	1934.956
CPO₂⁺	1550.28	1551.13	1556.97	1557.78	Eu⁺	175	189.1962	175	189.1962
N₂O⁺	1964.79	1987.89	1964.03	1987.10	Eu⁺	964.9762	979.1724	1103.125	1117.324
ArArH⁺	1203.25	1198.72	1203.25	1198.72	Eu⁺	1829.293	1843.492	1988.525	2002.724

Table (5): Reactions of arsenic with different gasses in dynamic reaction cell in ICP-MS*

The reactant	$\Delta_f H^\circ_{298}$	the products	$\Delta_f H^\circ_{298}$	$\Delta_f H^\circ_{298}$ difference
	KJ/mol		KJ/mol	KJ/mol
As ⁺ + CH ₃ F	1527.95	AsCH ₃ F ⁺	1327.76	-200.19
As ⁺ + CH ₃ F	1527.95	AsF ⁺ + CH ₃	1586.77	58.82
As ⁺ + CH ₃ F	1527.95	AsCH ₂ ⁺ + HF	1496.68	-31.27
As ⁺ + CH ₃ F	1527.95	AsCHF ⁺ + H ₂	1556.85	28.89
As ⁺ + CH ₃ F	1527.95	CH ₂ F ⁺ + As H ⁺	1580.75	52.80
Ar ⁺ + 1/2 Cl ₂	1536.82	ArCl ⁺	1274.09	-262.73
As ⁺ + 1/2 O ₂	1427.50	AsO ⁺	1310.28	-117.22
2 ArCl ⁺ + H ₂	2686.86	2Ar ⁺ + 2HCl	3007.78	320.93
As ⁺ + N ₂ O	2145.99	AsO ⁺ + N ₂	1831.26	-314.72

* CBS-Q method of calculation is used for these calculations reactions are exothermic reactions.

The last product of this reaction is CH₂F⁺ + AsH⁺ ($\Delta_f H^\circ_{298} = 52.80$ KJ/mol) which is an endothermic reaction, according to the hydride transfer. These different reactions show that two exothermic processes may occur between As⁺ and CH₃ as the formation of AsCH₃F⁺ ($\Delta_f H^\circ_{298} = -198.15$ kJ/mol) and AsCH₂⁺ + HF ($\Delta_f H^\circ_{298} = -34.42$ kJ/mol) and the two exothermic cases are suggested to be the favored reaction product ions during measuring

process. As mentioned before the main problem of interferences comes from ⁴⁰Ar³⁵Cl⁺ which has the same mass of As. Ar Cl is a product of the reaction Ar⁺ + 1/2 Cl₂ → ArCl⁺ ($\Delta_f H^\circ_{298} = -262.73$ kJ/mol), and this reaction is exothermic reaction and it is easy to occur making the interference with arsenic, so, ArCl signal can be decreased by adding H₂, which cause the reduction of ArCl according the reaction 2ArCl⁺ + H₂ → 2Ar⁺ + 2HCl

($\Delta_f H^\circ_{298} = 320.93$ kJ/mol). As we see this reaction is endothermic reaction and the needed activation energy to complete the reaction can be obtained from the plasma. Arsenic can also be switched to AsO^+ ($m/z = 91$) which can be measured far from $ArCl$ ($m/z = 75$). And this process can be completed using oxidizing agent like O_2 or N_2O according to the reactions $As^+ + \frac{1}{2} O_2 \rightarrow AsO^+$ ($\Delta_f H^\circ_{298} = -117.22$ kJ/mol) and $As^+ + N_2O \rightarrow AsO^+ + N_2$ ($\Delta_f H^\circ_{298} = -314.72$ kJ/mol), respectively. It is clear that the last two reactions are exothermic reactions.

Conclusion

In this work Gaussian 09 is used for calculating thermo chemistry of species ($^{40}Ar^{35}Cl^+$, $^{59}Co^{16}O^+$, $^{36}Ar^{38}Ar^1H^+$, $^{38}Ar^{37}Cl^+$, $^{36}Ar^{39}K^+$, $^{150}Nd^{++}$, $^{150}Sm^{++}$ and $^{150}Eu^{++}$) which interfere with arsenic in ICP-MS. The species ($AsCH_3F^+$, AsF^+ , $AsCH_2^+$, $AsCHF^+$ and AsO^+), that are obtained from the reactions between arsenic and different gases which are common used in DRC-ICP-MS using G3 and CBS-Q methods of calculations except ($^{150}Nd^{++}$, $^{150}Sm^{++}$ and $^{150}Eu^{++}$) are calculated using MP2/CEP-4G and MP3/CEP-4G methods. Proton affinity of $^{36}Ar^{38}ArH^+$ and $^{40}Ar^{34}SH^+$ are calculated and gave values 326.112 and 866.742, respectively.

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