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THERMODYNAMIC PARAMETERS OF WELL WATER IN BABYLON GOVERNORATE OF IRAQ

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Abstract

A study was conducted Water samples were collected from different areas of Babylon Governorate to describe the water from the thermodynamic side depending on the activity of some ions and ion pairs in the Groundwater. The ionic strength and the efficiency factor were also calculated to calculate the activity. Laboratory tests were carried out for water, which included water salinity as well as concentration of ions. It was found that the highest activity of ions was in the areas of Hashmeeh 1, Hashmeeh 2, Al-Madhatyh and Al-Kfel by 76.75, 74.45 and 74.4 mmol.L^{-1} respectively the sodium ion activity, which exceeded the chloride ion, which in turn exceeded the calcium ion, which also surpasses the magnesium and finally came the effectiveness of potassium. The ion pairs measured and we found the highest value of the ionic [$CaSO_4$] o were also detected for the desalinated water and reached 5.76 mmol.L^{-1} For the ion pairs [$MgSO_4$] the highest value of the water was 1.22 mmol.L^{-1} for Al-Kfel1. It is show from the above that the effect of activity ions and their ion pairs is highly correlated with the concentration of ions and the degree of electrical conductivity.

Keywords **:** ionic strength, ion activity, thermodynamic, ion pairs

Introduction

There is a great need to study thermodynamic parameters to describe the water of wells in Babylon Province to accurately reflect the existence of positive and negative ions, the ion activity and ion pairs. Lindsay (1979) states that, the ion activity is the result of two factors, namely the efficiency and concentration of the ion being studied. Groundwater is an important water resource in the desert and semi-desert areas of the world in general and in Iraq in particular because it compensates for the shortage of water in these areas and is of great importance during the summer when water shortage during agriculture Groundwater moves slowly through the soil compared to the surface flow of rainwater. (Hassan *et al*., 2019). Many studies (Boit and Bruggenwen, 1981), in their study of ion-value solutions, they found that the ion efficiency coefficient in these solutions is equal and approaching one at dilution. Ion pairs is a good bonding and bonding between opposite charges. When ionic coupling is formed, the water molecules surrounding the ion are not removed. The ion pairs is calculated based on the coefficient of efficiency, ionic strength and efficiency. The ionic water structure contributes to ionic pairs (Esmail, 2001 and Alani, 2005) Bohn *et al*. (1985) noted that when the positive and negative ions in the solution converge to a distance of less than 5 μm, there will be a force of attraction and thus the coupling of the ions and their coupling by force During this bondage, the ions retain their aquatic layer and this phenomenon is called ion pairs.

(Wright, 2005) three types of ionic coupling:

1 - Ion pairs formed

2 - Ionic duality with full interruption.

3 - Ionic duplication with partial interruption.

Adams (1971) summarized the basic principles of ion pairs (Wolt, 1988), a program for estimating the value of ion pairs, concentration and effectiveness in water.

Materials and Methods

20 wells were selected in different areas and distributed in Babil Governorate. The samples were collected and transferred to the laboratory after conducting some of the following tests (such as electrical conductivity, pH). The positive ions of calcium, magnesium, sodium and potassium were measured as soluble positive ions and sulphates, chlorides, carbonates, The ionic strength was calculated by using the equation

I=EC*0.013

I= ionic Strength

Ec = electrical conductivity

The efficiency coefficient was then calculated using the equation :

Log fi= - A ZI2√I/(1+Bdi√I)), A is 0.509 at 25 Cº, B is 0.3285 at 25 Cº , Zi is Ionic charge and d is Ion size parameter.

a= fi * ci

a= ion activity

The proposed Excel program (Abed, 2002) was used to calculate the ion pairs, free ions and ionic strength in the water under study. Some Equation and measured get by using (Kim *et al*., 2013 and Sposito, 2008).

Table 1 : show some property for the water of well under study.

	Y	X	EC (µs/cm)	Ph	Depth(m)
Eskan	32.482694	44.432333	3380	7.41	12
Jamaeh	32.462000	44.420389	7920	7.13	9
Babylon University	32.405889	44.400278	6160	7.18	10
Babylon University 2	32.398111	44.396111	5280	7.4	12
AlMohandseen	32.448806	44.392806	17570	7.31	9
AlNeel	32.546000	44.540750	3680	7.18	7
Ameh Basha	32.656694	44.571389	1963	7.22	14
Khatwneh 2	32.627278	44.468750	6090	7.33	10
Khatwneh 1	32.621361	44.463806	1688	7.22	12
AlBoor	32.576694	44.577389	2830	7.15	10
AlMahaweel 1	32.644889	44.395417	1518	7.41	12
AlMahaweel 2	32.640361	44.377194	12310	7.62	9
AlMahaweel 3	32.673167	44.429778	4250	7.18	12
AlRestmeh	32.302333	44.464972	1814	7.41	10.5
AlKfel 1	32.209028	44.371917	23000	7.11	12
AlKfel 2	32.250583	44.428250	7600	7.12	12
AlKfel 2	32.348528	44.381056	2430	7.77	10
AlKfel 3	32.379583	44.363639	1939	7.44	9
Abo Ghark	32.466500	44.343250	10190	7.33	11
Madhatyh	32.398639	44.667806	34700	7.11	9
Hashmeeh1	32.447917	44.873222	50200	7.12	9
Hashmeeh2	32.487694	44.949806	28300	7.3	9
Hashmeeh3	32.533194	44.990194	3000	7.14	9
Shomali	32.320722	44.905056	3140	7.15	7.5

Result and Discussion

Ion activity

From the table on the effectiveness of the ions and the shapes shown, there is a high variation between the activity of the ions and the variation between the selected areas under study.

$$K < Mg < Ca < HCo_3 < Cl < Na$$

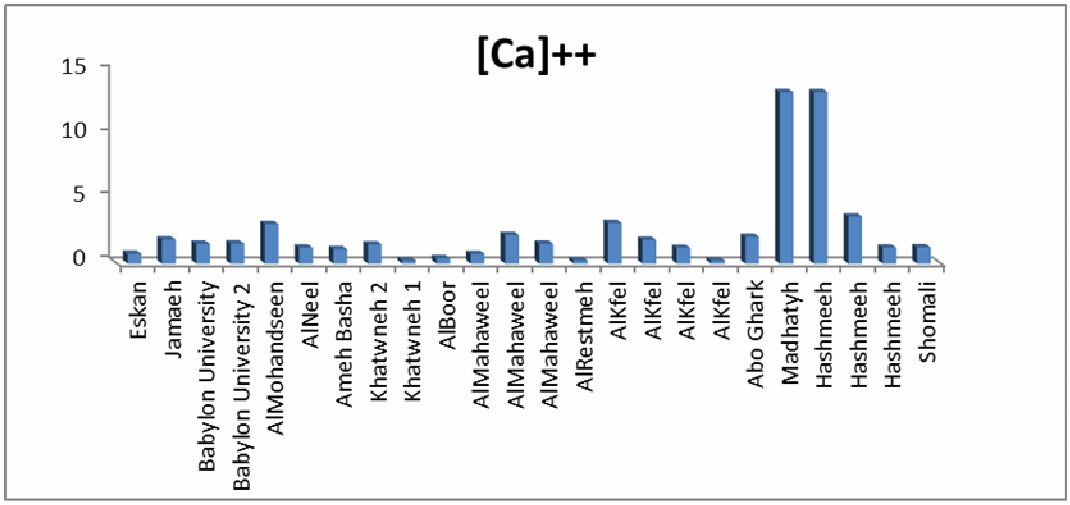
It is found that the highest efficiency is sodium ions followed by ion chloride and then bicarbonate followed by calcium and magnesium and the latest ion ion potassium. This arrangement is based on the contribution of ions in the formation of ion pairs and its correlation.

For sodium, the highest value in the waters of the Hashmeeh 1 area was 76.28 mmol.L^{-1}, followed by the water of the wells of Madhtyh 76.18 mmol.L^{-1} and Hashmeeh 2 73.22 mmol.L^{-1}, followed by the water of Al-Kefal 1, 66.97 mmol.L^{-1}. As for chloride, the highest value was in the water of the well of Hashmeeh 2, followed by the soil of Madhtyh and Al- Hashmeeh 1, followed by Al-Kfel 1 soil (76.75, 74.45, 74.22 and 67.90) mmol.L^{-1} respectively. The lowest efficiency of chloride ion was in Al-Restmeh water at 3.92 mmol.L^{-1}. In the ionic activity of the bicarbonate, the highest value was 25.06 mmol.L^{-1} in the well of Hashmeeh 1, followed by the soil of Madhtyh 23.32 mmol.L^{-1} and the Hashmeeh well 2 by 22.75 mmol.L^{-1}. The lowest water in the Bicarbonate was Al-Mahaweel water 1.4. 13.36, 13.36, 3.6 and 3.1) mmol.L^{-1} for the water of Hashmeeh wells 1, Madhtyh, Hashmeeh 2 and Al-Kfel 1 respectively, and so for the rest of the water, In the magnesium ion activity, the highest values were found (3.16, 3.14, 2.65 and 2.58) mmol.L^{-1} for the water of the wells of Madhtyh, Hashmeeh 1, Al-Kfel 1 and Al-Mohandsin respectively, and so for the rest of the water. In the sulfur ion activity, the highest values were found (13.36, 13.36, 3.6 and 3.1) mmol.L^{-1} mmol.L^{-1} for the wells of Hashmeeh 2, Al-Kfel 2, Abi Ghark and Al-Mahaweel 2 respectively, and so on for the rest of the

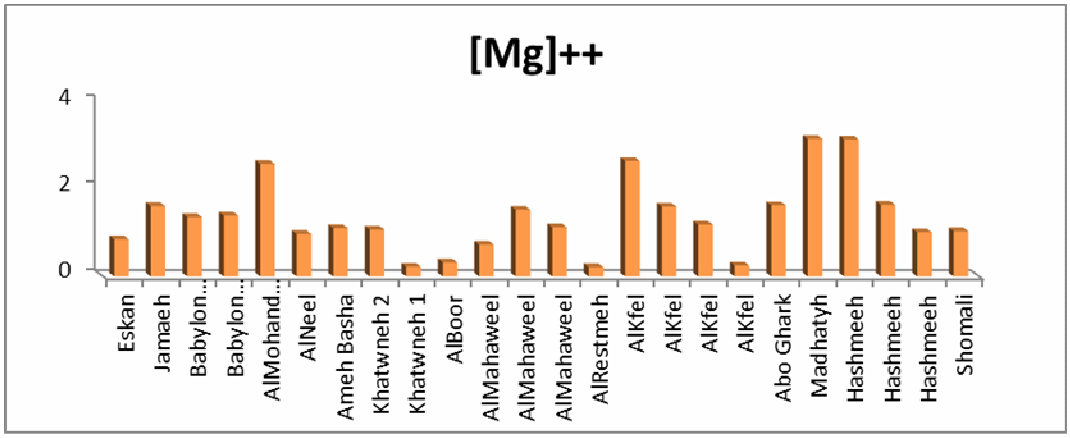
water to reach the lowest value in the waters of the Kfel 4 area by 0.87 mmol.L^{-1}. The lowest values in the efficiency of ions were the potassium ions with the highest value in the Hashmeeh soil 1 by 4.10 mmol.L^{-1} and Madhtyh of 4.03 mmol.L^{-1} and the lowest value in the water well housing by 0.022 mmol.L^{-1}.

This is due to the variation in the activity of the electrical conductivity of each region in addition to the concentration of the element in this water, which is an effect on the values of the ionic force and the efficiency coefficient, which in turn is reflected in the efficiency of the ions and the ionic (salih,2008 and Mam Rasool, 2000)

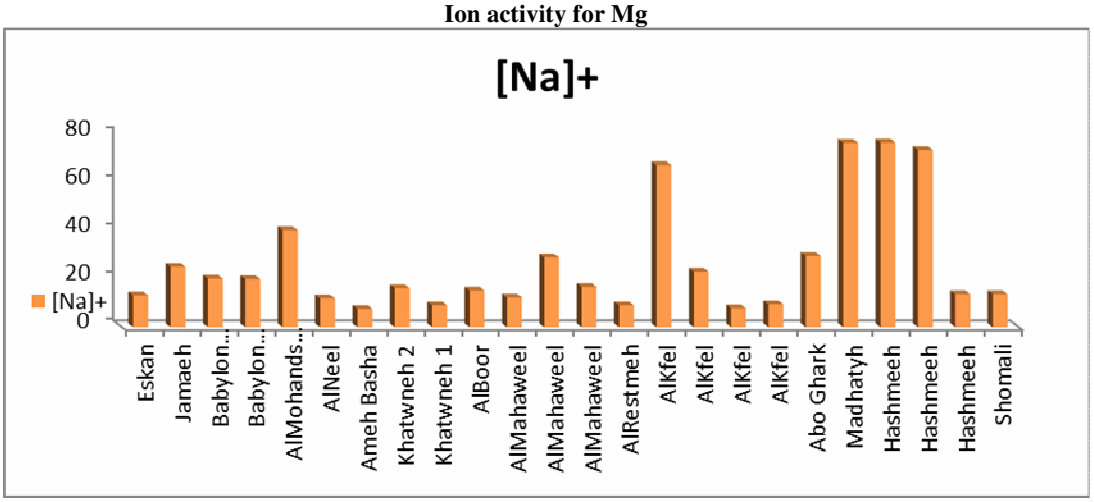
	$[MgHCO_3]^+$	$[CaHCO_3]^+$	$[KSO_4]^-$	$[NaSO_4]^-$	$[MgSO_4]^o$	$[CaSO_4]^o$
Eskan	0.064	0.072	0.000	0.081	0.216	0.217
Jamaeh	0.160	0.231	0.004	0.263	0.695	0.899
Babylon University	0.125	0.176	0.003	0.212	0.588	0.736
Babylon University 2	0.128	0.179	0.044	0.207	0.593	0.741
AlMohandseen	0.585	0.873	0.035	0.458	1.204	1.603
AlNeel	0.082	0.129	0.003	0.061	0.205	0.288
Ameh Basha	0.063	0.080	0.001	0.026	0.156	0.176
Khatwneh 2	0.100	0.175	0.035	0.134	0.365	0.572
Khatwneh 1	0.010	0.014	0.001	0.034	0.035	0.044
AlBoor	0.019	0.029	0.003	0.078	0.069	0.095
AlMahaweel1	0.015	0.019	0.005	0.077	0.186	0.214
AlMahaweel2	0.232	0.424	0.023	0.331	0.720	1.174
AlMahaweel3	0.114	0.195	0.046	0.153	0.424	0.649
AlRestmeh	0.009	0.013	0.001	0.033	0.032	0.042
AlKfel1	0.544	0.815	0.040	0.757	1.222	1.635
AlKfel2	0.166	0.239	0.009	0.269	0.769	0.987
AlKfel3	0.091	0.117	0.001	0.029	0.184	0.212
AlKfel4	0.010	0.012	0.001	0.036	0.040	0.041
Abo Ghark	0.218	0.348	0.030	0.342	0.776	1.107
Madhatyh	1.069	5.669	0.082	0.708	1.199	5.678
Hashmeeh1	1.143	6.092	0.083	0.709	1.194	5.678
Hashmeeh2	0.539	1.504	0.098	0.926	0.851	2.119
Hashmeeh3	0.061	0.092	0.001	0.094	0.287	0.387
Shomali	0.063	0.095	0.001	0.091	0.282	0.379



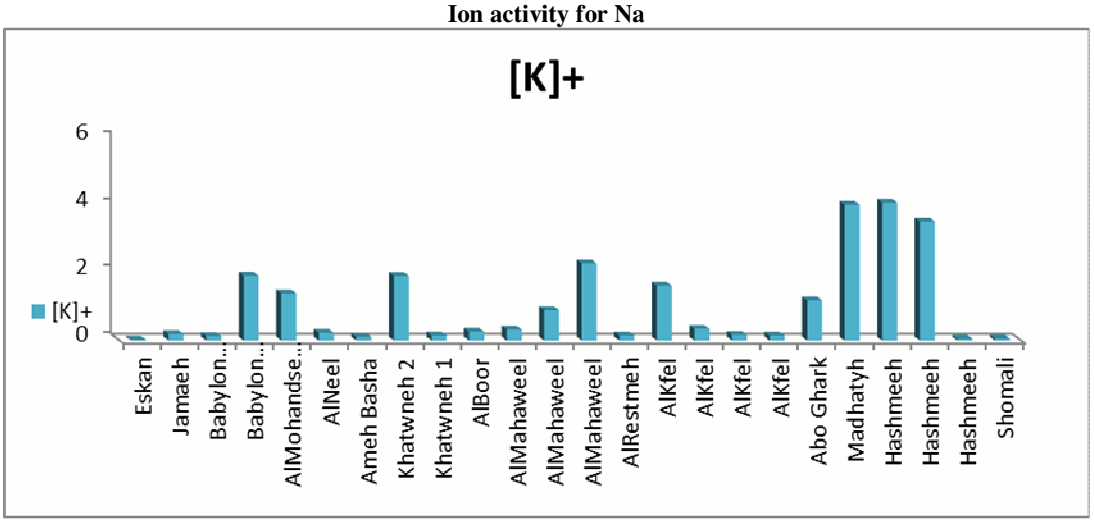
Ion activity for Ca



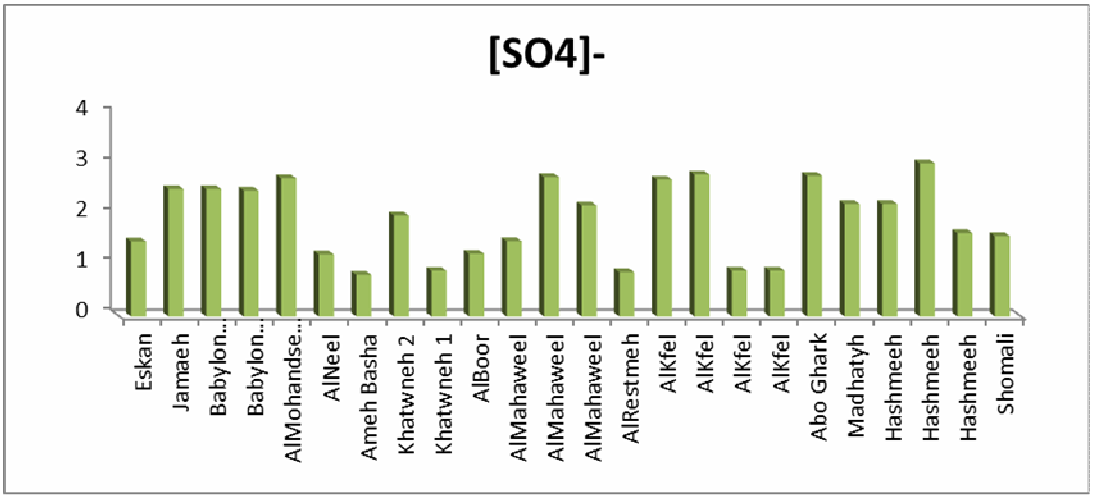
Ion activity for Mg



Ion activity for Na



Ion activity for K



Ion activity for So_4

Ion Pairs

Ion Pairs of the water of the sites under study has been identified as double ions $[CaSO_4]o$, $[MgSO_4]o$, $[NaSO_4]$ - and $[KSO_4]$ - and $[CaHCO_3]$ + and $[MgHCO_3]$.

	$[MgHCO_3]^+$	$[CaHCO_3]^+$	$[KSO_4]^-$	$[NaSO_4]^-$	$[MgSO_4]^o$	$[CaSO_4]^o$
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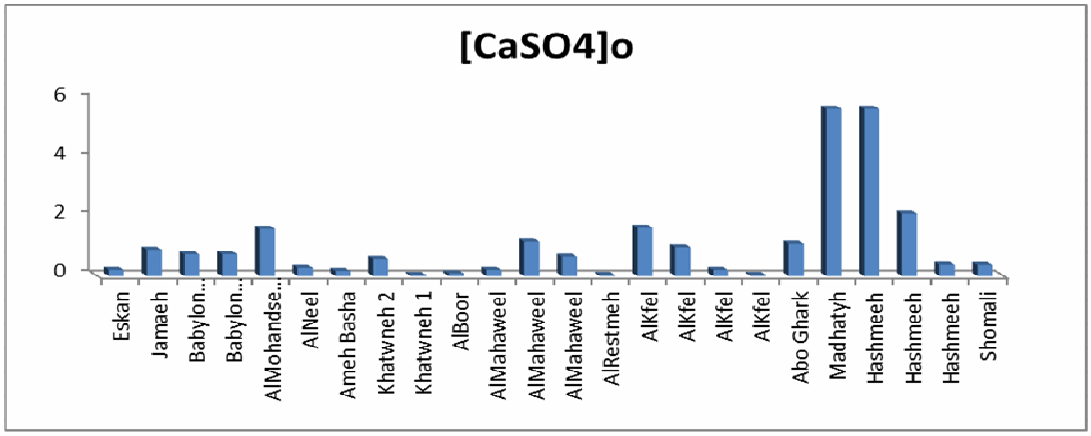
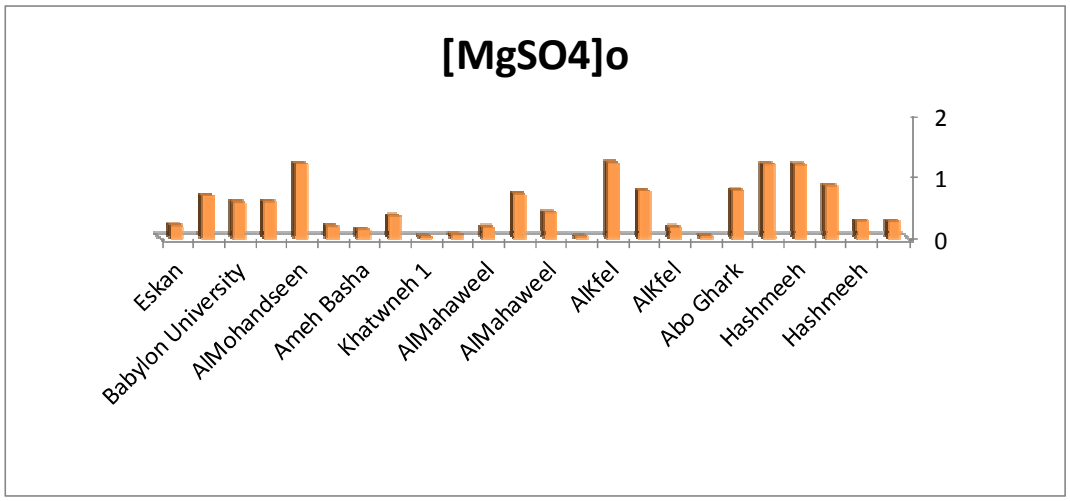
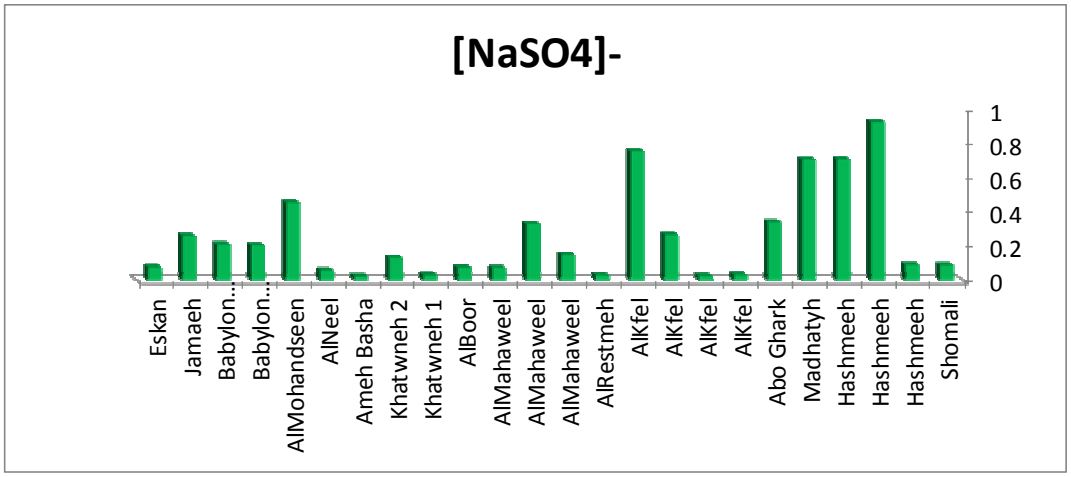


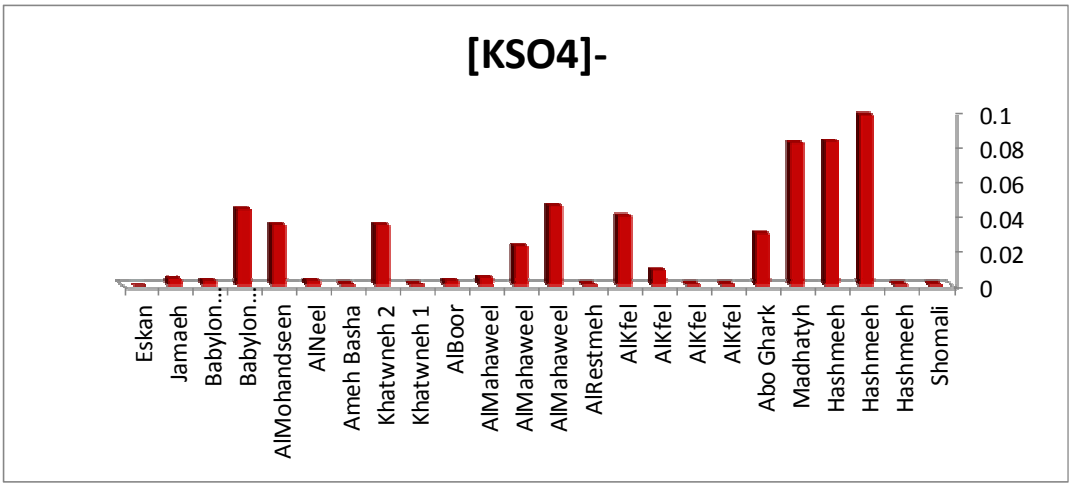
Ion pairs for $CaSO_4]o$



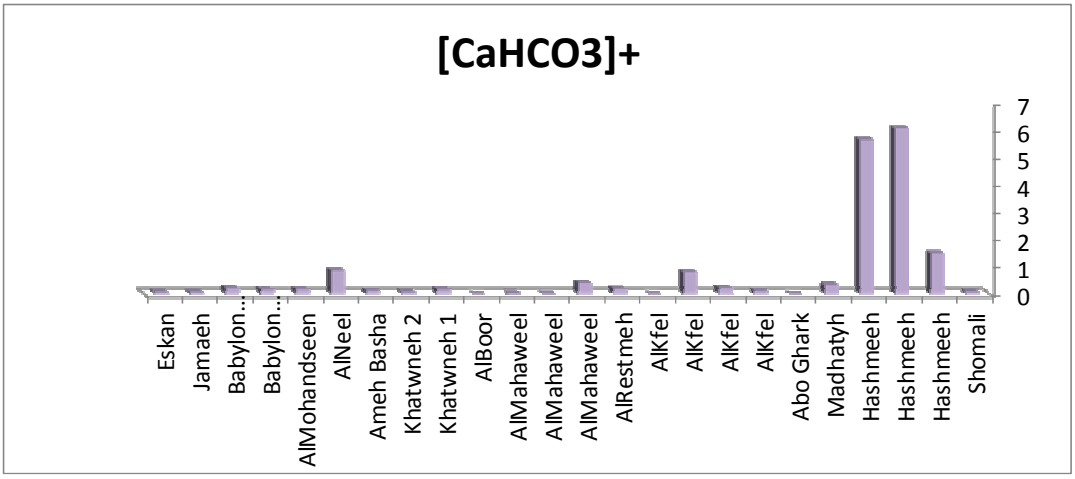
Ion pairs for $MgSO_4]o$



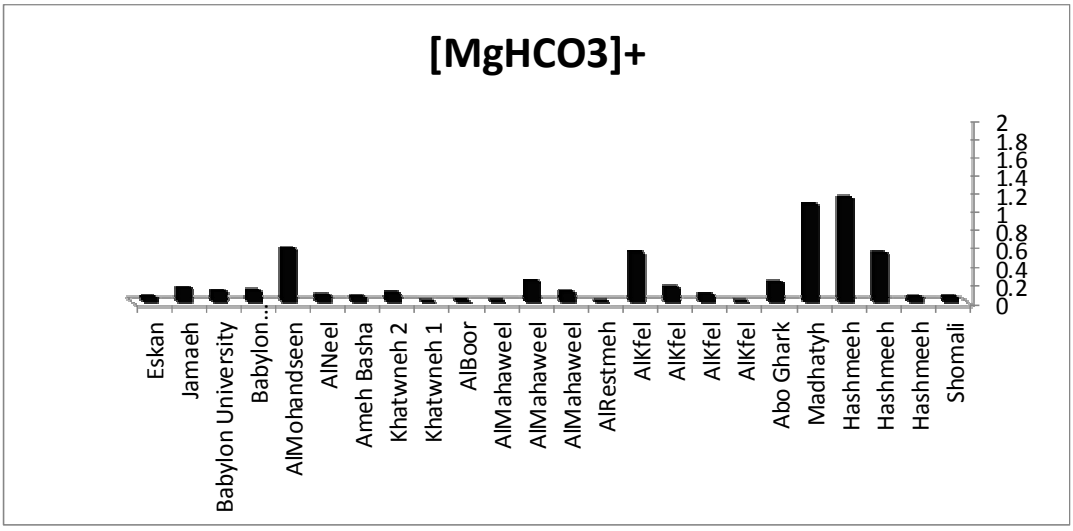
Ion pairs for $NaSO_4]-$



Ion pairs for $KSO_4]$-



Ion pairs for $[CaHCo_3]_+$



When we show the ion pairs for **$[CaSO_4]^o$** The highest values (5.67, 5.67, 2.11) mmol.L^{-1} were found for the madhtyh and Hashimeeh cultivars 1 and 2 respectively, while the lowest values were for kfel 4 by 0.041 mmol.L^{-1}. As for the ionic pairs [MgSO4] o, it was the highest values in the dependent areas Kfel 1 was 1.22 mmol.L^{-1}, then Al- Restamieh by 1.20 mmol.L^{-1} for madhtyh by 1.19 mmol.L^{-1} and Hashmiyah 1 also by 1.19 mmol.L^{-1}. Thus, for the rest of ion pairs, they were shown in tables and shapes. This difference is due to the ions and their effectiveness (Abdel Kadhim, 2013; Abdel Kadhim, 2016 and mohammed, 2018).

Selected Ion Pair Reactions and Their Equilibrium Constants

Ion Pairs	K_{eq}
$CaCO_3^o \leftrightarrow Ca^{2+} + CO_3^{2-}$	6.3×10^{-4}
$CaNO_3^+ \leftrightarrow Ca^{2+} + NO_3^-$	5.25×10^{-1}
$CaSO_4^o \leftrightarrow Ca^{2+} + SO_4^{2-}$	5.25×10^{-3}
$MgSO_4^o \leftrightarrow Mg^{2+} + SO_4^{2-}$	5.88×10^{-3}
$NaSO_4^- \leftrightarrow Na^+ + SO_4^{2-}$	2.4×10^{-1}
$NaCO_3^- \leftrightarrow Na^+ + CO_3^{2-}$	5.35×10^{-2}
$NaHCO_3^o \leftrightarrow Na^+ + HCO_3^-$	0.178×10^{-1}

Source : Davies, C.W. Ion Association, Butterworth, Washington, DC, 1962; Garrels, R.M., and C.L. Christ. Solutions, Minerals, and Equilibria, Harper & Row, New York, 1965.

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