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Crystal structure and chemical thermodynamic properties of potassium D-gluconate K(D-C$_6$H$_{11}$O$_7$)(s)

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Abstract An important coordination compound potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s) has been synthesized by liquid phase method. The chemical component and crystal structure of the important compound are characterized by chemical analysis, elemental analysis, and X-ray crystallography. Single-crystal X-ray analysis reveals that the compound exhibits the chelate property of D-gluconate anions to K$^+$ cations, a six-membered chelate ring is formed by the coordination of K$^+$ with O2 of carboxylate and O4 of hydroxyl in a D-gluconate, and one cation is coordinated to six D-gluconate anions. The lattice potential energy and ionic volume of the anion [D-C$_6$H$_{11}$O$_7$]$^-$ are obtained from crystallographic data. In accordance with Hess' law, a reasonable thermochemical cycle is designed according to the practical synthesis reaction of the compound and the standard molar enthalpy of formation of the compound is calculated to be $-(1754.17 \pm 0.19)$ kJ mol^{-1} as an important physical quantity in chemical thermodynamics by an isoperibol solution–reaction calorimeter. Molar enthalpies of dissolution of the compound at various molalities are measured at $T = 298.15$ K in the double-distilled water. According to Pitzer's electrolyte solution theory, molar enthalpy of dissolution of the title compound at infinite dilution is calculated to be $\Delta_s H_m^\infty = (27.92 \pm 0.21)$ kJ mol^{-1}. In terms of the above value, the standard molar enthalpy of formation of the anion [D-C$_6$H$_{11}$O$_7$]$^-$ in the aqueous solution is determined to be $= -(1473.87 \pm 0.28)$ kJ mol^{-1}. The values of relative apparent molar enthalpies ($^\Phi L$) and relative partial molar enthalpies of the solvent ($\bar{L}_1$) and the compound ($\bar{L}_2$) at different concentrations $m/(\text{mol kg}^{-1})$ are derived from the experimental values of the enthalpies of dissolution of the compound.

Introduction

It is well known that D-glucose is one of the most important and basic nutrients. It is often applied to supplement nutrition and energy for some patients who lack vitamins. More importantly, it is used as one of the carbon and energy sources in the human body and maintains the normal physiological and biological functions for human body. There is an aldehyde group at the end of the D-glucose molecule, which is easily oxidized to D-gluconic acid. The latter can be easily combined with many inorganic metal ions such as K$^+$, Na$^+$, and Ca^{2+}. Many bioactive coordination compounds are produced under the weak basicity at pH 7.4 in the body fluid, and the body fluid acid–base balance is maintained, which have an important influence on the growth and development of the human body. In the past decades, D-gluconic acid series products are widely used as nutrient additives in food, medicine and

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pharmaceutical industry [1–3] due to the coordination properties of D-gluconate anions to metal ions. In recent years, as an important nutritional supplement, D-gluconate is easily absorbed by the human body and a great attention is paid to it by people all over the world because it is non-toxic, fully biodegradable and can be used as new generation of biological metal supplements. For these reasons, it is very useful to study the crystal structures and electrolyte solution properties of D-gluconates to develop their new application fields and to carry out relevant theoretical research.

Potassium is one of the important elements necessary for the human body. K^+ cation as prosthetic group of some enzymes can promote the activity of enzyme in cells. It can also stabilize internal structure of cells and involve in protein synthesis. Potassium is an essential part of most organisms and plays a very important role in the process of neural information transfer. Both of potassium ion and sodium ion form a "Na–K pump." It can adjust the balance of potassium and sodium in the body. "Limit sodium, supplement potassium" is the basis to prevention and treatment of high blood pressure. When too much potassium is lost from body, it will lead listless, agitated mood and even death [4]. Potassium D-gluconate can serve as a good potassium supplement agent, it is soluble in the body liquid, and it is easily absorbed by human body.

Thermodynamic properties of the substances are one of the most important physical quantities in science and technology [5–12]. In this paper, we report the crystal structure of an important coordination compound potassium D-gluconate $K[D-C_6H_{11}O_7](s)$. And the lattice potential energy and ionic volume of the common anion are obtained from crystallographic data. The molar enthalpies of dissolution of reactants and product in the designed reaction are determined by an isoperibol solution–reaction calorimeter. The standard molar enthalpy of formation of potassium D-gluconate $K[D-C_6H_{11}O_7](s)$ is determined based on these calorimetric experimental results. Molar enthalpies of dissolution of potassium D-gluconate $K[D-C_6H_{11}O_7](s)$ at various molalities are measured at $T = 298.15$ K in the double-distilled water. According to Pitzer's theory, the molar enthalpy of dissolution of the title compound at infinite dilution is obtained. The values of relative apparent molar enthalpies ($^\Phi L$), relative partial molar enthalpies ($\bar{L}_2$) of the compound and relative partial molar enthalpies ($\bar{L}_1$) of the solvent (water) at different concentrations $m/(\text{mol kg}^{-1})$ are derived from the experimental values of the enthalpies of dissolution of the compound.

Experimental

Preparation of the title compound

The provenances and purities of the chemicals used in the synthesis and calorimetric experiments are shown in Table 1. The compound is prepared by concentrating aqueous solution of D-gluconolactone and potassium hydroxide (molar ratio 1: 1) in water for 2 h. When the final solution is cool, excessive ethanol is added to the solution. And the colorless single crystals suitable for X-ray diffraction are obtained 5 days later by slow evaporation. The sample is placed in a vacuum desiccator at $T = 303.15$ K to dry in vacuum for 24 h, and the final product is placed in weighing bottles and preserved in the desiccator. The chemical composition of the compound is analyzed by element analyzer (model: PE-2400 II, PerkinElmer, USA) under "C–H–N mode" and "O mode." The element analyzer used in our research has three kinds of analytical modes: "C–H–N mode", "C–H–N–S mode" and "O mode." The content of the oxygen element is analyzed exactly under the "O mode." The contents of the carbon and hydrogen elements are obtained by the H–C–N mode. At last, the mass fraction purity of the C, H, and O is determined by elemental analyzer. The percentage of potassium K can be analyzed by chemical analysis, and the values (calculated for $K[D-C_6H_{11}O_7]$: C 30.76, H 4.74, O 47.81, K 16.69%; found: C 30.77, H 4.75, O 47.82, K 16.66%, respectively.) show that the mass fraction purity of the compound is >0.998.

Crystallographic data collection and refinement

Single-crystal structure analysis of the compound is performed on a Bruker Smart 1000 diffractometer with a CCD detector with Mo-Kα radiation ($\lambda = 0.071073$ nm). The intensity data are collected in the φ–ω scan mode at $T = (298 \pm 2)$ K. The empirical absorption corrections are based on multi-scan. The structure is solved by direct method using SHELXTL and difference Fourier syntheses, and all non-hydrogen atoms are refined anisotropically on F^2 by full-matrix least-squares technique using the SHELXTL-97 program package. The hydrogen atoms are added theoretically, riding on the concerned atoms, and not refined. The final full-matrix least-squares refinement on F^2 is applied for all observed reflections [$I > 2\sigma(I)$]. All calculations are made with the program package SHELXTL [5, 6]. We have applied for a CCDC 888208 for potassium D-gluconate $K[D-C_6H_{11}O_7](s)$.

Table 1 The provenances and purities of the chemicals used in the synthesis and calorimetric experiments

Chemicals	Provenances	Purities (mass%)
D-Gluconolactone	J&K Scientific Ltd, China	99.5
Potassium hydroxide	J&K Scientific Ltd, China	99.99
Anhydrous ethyl alcohol	Tianjin No.3 Chemical Reagent Factory, China	99.5
Potassium D-gluconate	Prepared by our laboratory	>99

Isoperibol solution–reaction calorimeter

The isoperibol solution–reaction calorimeter consists primarily of a precision temperature controlling system, an electric energy calibration system, a calorimetric body, an electric stirring system, a thermostatic bath made from transparent silicate glass, a precision temperature measuring system, and a data acquisition and processing system. During whole experiment, the water thermostat is automatically maintained at $T = 298.15$ K and the maximum variation is found to be $\pm 1 \times 10^{-3}$ K. Experiments have demonstrated that the precision of measuring the temperature can reach $\pm 1 \times 10^{-4}$ K. The principle and structure of the calorimeter are described in detail elsewhere [5, 6].

The reliability of the calorimeter is verified previously by measuring the molar enthalpy of dissolution of KCl (calorimetrically primary standard) in the double-distilled water. According to the molar ratio of KCl to water, $n_{KCl} : n_{H_2O} \approx 1 : 1110$, a certain amount of KCl is dissolved in 100 cm^3 of double-distilled water at $T = (298.15 \pm 0.001)$ K. The average enthalpy of dissolution of KCl is $(17,547 \pm 13)$ J mol^{-1}, which compares with corresponding published data $(17,536 \pm 3.4)$ J mol^{-1} under the same experimental conditions [13]. Experiments demonstrate that the uncertainty between the measuring value and the literature value is within $\pm 0.30\%$ [5, 6].

Results and discussion

Description of crystal structure

The molecular structure of the compound is plotted in Fig. 1. A summary of crystallographic data and refinement parameter is listed in Table 2. The selected bond lengths and angles of the title compound are listed in Table 3. From Table 2, it is found that the crystal system of K[D-C$_6$H$_{11}$O$_7$](s) is orthorhombic, the space group is P2(1)2(1)2(1), unit cell dimensions are $a = 0.50350(6)$ nm, $b = 0.74224(8)$ nm, $c = 2.3517(2)$ nm, $\alpha = \beta = \gamma = 90°$ and $Z = 4$.

Single-crystal X-ray analysis reveals that in each one molecule of K[D-C$_6$H$_{11}$O$_7$](s), the conformation of the D-gluconate anion is a six-member zigzag carbon chain which is nearly planar (see Fig. 1). The conformation is
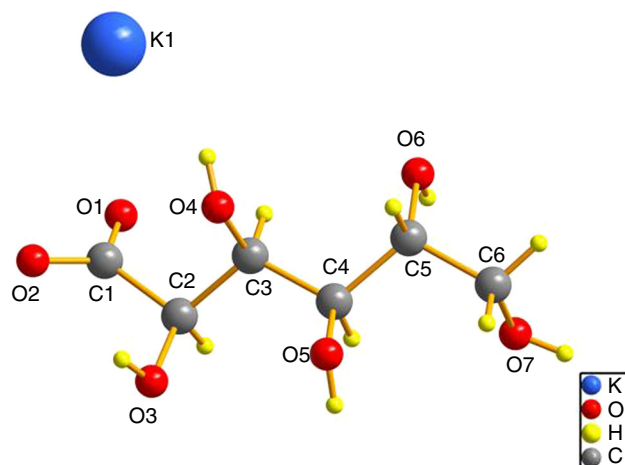

Fig. 1 Molecular structure in crystallographic independent unit of potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s)

essentially as same as what found in the studies [14, 15] about the crystal structures of potassium D-gluconate, rubidium D-gluconate and lead(II) D-gluconate, where the gluconate ion is almost fully extended and its six carbon atoms lie approximately in a common plane.

A six-membered chelate ring is formed by the coordination of K$^+$ with O2 of carboxylate and O4 of hydroxyl in a D-gluconate. The environment of the D-gluconate ligand bonding to the alkali metal ion (K$^+$ cation) and the ion-numbering scheme is shown in Fig. 2. In the title compound, each cation coordinates with six anions through hydroxyl oxygen and carboxylate oxygen, and each D-gluconate anion coordinates with six cations through hydroxyl oxygen and carboxylate oxygen (see Fig. 2). Thus, each alkali metal cation (K$^+$ cation) is coordinated to only one D-gluconate anion, and the coordination compound consists of one crystallographic independent alkali metal cation and one D-gluconate anion. And each cation is surrounded by a shell composed of oxygen atoms. The framework diagrams illustrating the coordination polyhedron of the title compound is given in Fig. 3.

The distances of carboxylate oxygens to the metal cation are very close (see Table 3), lying in the range 0.2660(2)–0.2913(2) nm for K[D-C$_6$H$_{11}$O$_7$]. The distances of hydroxyl oxygen to K$^+$ cation are lying in the range 0.2748(2)–0.3024(2) nm. The C–C bond lengths range from 0.1507(4) to 0.1534(4) nm for K[D-C$_6$H$_{11}$O$_7$], the C–OH bonds from

Table 2 Summary of crystallographic data and refinement parameters for potassium D-gluconate K[D-$C_6H_{11}O_7$](s)

Properties	Crystallographic data and refinement parameters
Empirical formula	$C_6H_{11}O_7K$
Formula weight	234.25
Temperature/K	298 ± 2
Wavelength/nm	0.071073
Crystal system	Orthorhombic
Space group	$P2(1)2(1)2(1)$
Unit cell dimensions/nm or °	$a = 0.50350(6)$
	$b = 0.74224(8)$
	$c = 2.3517(2)$
	$\alpha = 90$
	$\beta = 90$
	$\gamma = 90$
Volume/nm^3	0.87886 (16)
Z	4
Calculated density/g cm^{-3}	1.770
Absorption coefficient/ mm^{-1}	0.616
$F(000)$	488
Crystal size/mm^3	$0.38 \times 0.10 \times 0.08$
Theta range for data collection/°	2.88 to 25.02
Limiting indices	$-5 \leq h \leq 5, -8 \leq k \leq 8,$ $-27 \leq l \leq 8$
Reflections collected/unique	3969/1542 [R(int) = 0.0467]
Completeness to theta = 25.02/%	99.9
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9524 and 0.7996
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	1542/1/132
Goodness-of-fit on F^2	0.920
Final R indices [$I > 2$ sigma (I)]	$R_1 = 0.0357, wR_2 = 0.0775$
R indices (all data)	$R_1 = 0.0450, wR_2 = 0.0832$
Largest diff. peak and hole/ e nm^{-3}	290 and -258

Table 3 Selected bond lengths (nm) and bond angles (°) for potassium D-gluconate K[D-$C_6H_{11}O_7$](s)

Selected bond lengths/nm or angles/°			
K(1)–O(1)	0.2660(2)	C(4)–O(5)–H(5)	109.5
K(1)–O(2)#1	0.2793(2)	C(5)–O(6)–H(6)	109.5
K(1)–O(2)#2	0.2913(2)	C(6)–O(7)–H(7)	109.5
K(1)–O(4)#2	0.3024(2)	O(2)–C(1)–O(1)	124.2(3)
O(1)–C(1)	0.1251(3)	O(2)–C(1)–C(2)	119.5(3)
O(2)–C(1)	0.1252(3)	O(1)–C(1)–C(2)	116.2(3)
O(3)–C(2)	0.1409(3)	O(3)–C(2)–C(3)	114.9(3)
O(3)–H(3)	0.08200	O(3)–C(2)–C(1)	113.1(2)
O(4)–C(3)	0.1429(3)	C(3)–C(2)–C(1)	108.7(2)
O(4)–H(4)	0.08200	O(3)–C(2)–H(2)	106.5
O(5)–C(4)	0.1421(4)	C(3)–C(2)–H(2)	106.5
O(5)–H(5)	0.08200	C(1)–C(2)–H(2)	106.5
O(6)–C(5)	0.1416(4)	O(4)–C(3)–C(4)	110.5(2)
O(6)–H(6)	0.08200	O(4)–C(3)–C(2)	110.5(2)
O(7)–C(6)	0.1417(4)	C(4)–C(3)–C(2)	114.1(2)
O(7)–H(7)	0.08200	O(4)–C(3)–H(3A)	107.1
C(1)–C(2)	0.1531(4)	C(4)–C(3)–H(3A)	107.1
C(2)–C(3)	0.1531(4)	C(2)–C(3)–H(3A)	107.1
C(2)–H(2)	0.09800	O(5)–C(4)–C(3)	113.3(2)
C(3)–C(4)	0.1517(4)	O(5)–C(4)–C(5)	105.3(3)
C(3)–H(3A)	0.09800	C(3)–C(4)–C(5)	112.6(2)
C(4)–C(5)	0.1534(4)	O(5)–C(4)–H(4A)	108.5
C(4)–H(4A)	0.09800	C(3)–C(4)–H(4A)	108.5
C(5)–C(6)	0.1507(4)	C(5)–C(4)–H(4A)	108.5
C(5)–H(5A)	0.09800	O(6)–C(5)–C(6)	111.7(3)
C(6)–H(6A)	0.09700	O(6)–C(5)–C(4)	112.2(3)
C(6)–H(6B)	0.09700	C(6)–C(5)–C(4)	111.6(3)
O(1)–K(1)–O(2)#1	83.21(6)	O(6)–C(5)–H(5A)	107.0
O(1)–K(1)–O(2)#2	68.43(6)	C(6)–C(5)–H(5A)	107.0
O(2)#1–K(1)–O(2)#2	145.63(3)	C(4)–C(5)–H(5A)	107.0
O(1)–K(1)–O(4)#2	79.04(6)	O(7)–C(6)–C(5)	108.8(3)
O(2)#1–K(1)–O(4)#2	87.33(6)	O(7)–C(6)–H(6A)	109.9
O(2)#2–K(1)–O(4)#2	69.03(6)	C(5)–C(6)–H(6A)	109.9
C(1)–O(1)–K(1)	130.08(18)	O(7)–C(6)–H(6B)	109.9
C(2)–O(3)–H(3)	109.5	C(5)–C(6)–H(6B)	109.9
C(3)–O(4)–H(4)	109.5	H(6A)–C(6)–H(6B)	108.3

Symmetry codes: #1 $-x + 1, y - 1/2, -z + 1/2$; #2 $x + 1, y, z$

0.1409(3) to 0.1429(3) nm for K[D-$C_6H_{11}O_7$], and the differences from the means in lengths are within the limits of the experimental error. These results are in good agreement with those of the crystal structures in the normal D-gluconate salts. The differences are probably due to inaccuracy in the structure analysis and the different crystal surrounding for every atoms. The two C–O bonds in the carboxyl group are found to have lengths 0.1251(3) and 0.1252(3) nm for K[D-$C_6H_{11}O_7$]. The angles (see Table 3) O_1–C_1–C_2 and O_2–C_1–C_2 are 116.2(3)° and 119.5(3)° for

K[D-$C_6H_{11}O_7$], respectively. The carboxyl groups are symmetrical within experimental errors with an angle of 124.2(3)° between the two C–O bonds for K[D-$C_6H_{11}O_7$]. The differences are not significant. Similar differences are observed in many other determinations, but these always involve the different crystal forces for carboxylate oxygen.

Hydrogen bonds distances and angles are listed in Table 4. In the structure, there are six different O–O
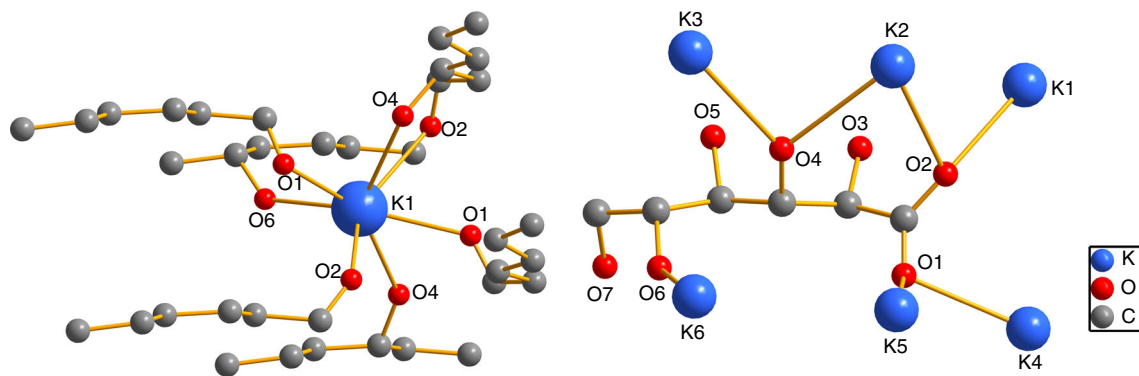
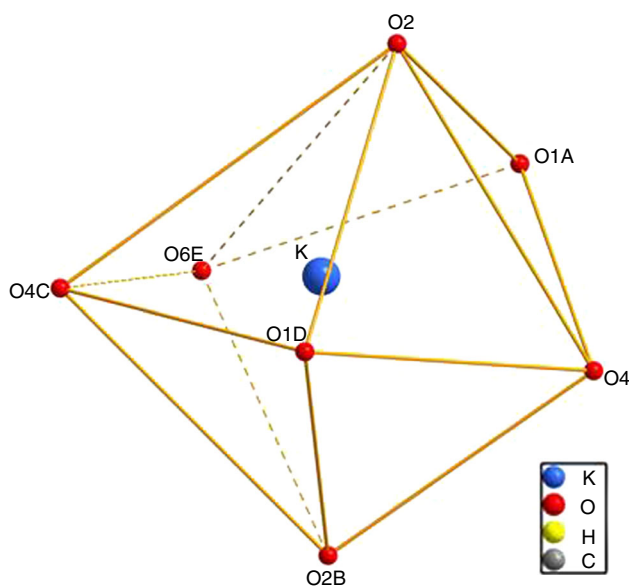**Fig. 2** The environment of the cations and anions for potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s)

Fig. 3 Framework diagram of the coordination polyhedron for potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s)

Table 4 Hydrogen bond lengths (nm) and bond angles (°) for potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s)

D–H···A	d(D-H)/ nm	d(H···A)/ nm	d(D···A)/ nm	<(DHA)/ °
O(3)–H(3)···O(1)#3	0.082	0.193	0.2726(3)	164.3
O(4)–H(4)···O(2)#1	0.082	0.196	0.2779(3)	175.8
O(4)–H(4)···O(1)#1	0.082	0.245	0.2991(3)	124.9
O(5)–H(5)···O(7)#4	0.082	0.203	0.2718(3)	140.9
O(6)–H(6)···O(5)#2	0.082	0.199	0.2759(3)	156.6
O(7)–H(7)···O(3)#5	0.082	0.197	0.2684(3)	145.0

Symmetry codes: #1 $-x + 1$, $y - 0.5$, $-z + 0.5$; #2 $x + 1$, y, z; #3 $x - 1$, y, z; #4 $x - 0.5$, $-y + 1.5$, $-z$; #5 $x + 0.5$, $-y + 1.5$, $-z$

distances shorter than 0.3 nm for K[D-C$_6$H$_{11}$O$_7$]. All the oxygen atoms of hydroxyl groups of the title compound participate in intermolecular hydrogen bonds utilizing all oxygen-bonded hydrogen atoms.

Lattice potential energy and ionic volume of D-C$_6$H$_{11}$O$_7^-$ anion

Equation (1) used to estimate lattice potential energy of generalized type of salt M_pX_q is obtained from the literature [16]:

$$U_{POT} = \sum n_i z_i^2 \left(\alpha'/V_m^{1/3} + \beta' \right) \tag{1}$$

where α' and β' are appropriate fitted coefficients chosen according to the stoichiometry of the salt, n_i is the number of ions with a charge z_i in the formula unit, and V_m is the molecular volume.

For the salts MX (1:1), MX_2 (1:2), and M_2X (2:1), Eq. (1) is changed to:

$$U_{POT} = |z_+||z_-|v\left(\alpha'/V_m^{1/3} + \beta' \right) \tag{2}$$

where z_+ and z_- are the respective charges on the cation and anion of the compound, v is the number of ions per molecule and equals $(p + q)$. In the case of the salt of formula MX with charge ratio (1:1) like K[D-C$_6$H$_{11}$O$_7$], $z_+ = 1$, $z_- = 1$, $p = 1$, $q = 1$, $v = 2$, $\alpha' = 117.3$ kJ mol^{-1} nm, $\beta' = 51.9$ kJ mol^{-1} [16], and V_m is in unit of nm^3 and expressed as follows:

$$V_m/\left(nm^3\right) = M_m/\rho N_A = 1.66045 \times 10^{-3} M_m/\rho \tag{3}$$

where N_A is Avogadro's constant, 6.02245×10^{23} molecule mol^{-1}, M_m is molar weight of the molecule, ρ is the density of the substance, and V_m(MX) is calculated to be 0.2198 nm^3 for K[D-C$_6$H$_{11}$O$_7$] from Eq. (3). Thus, Eq. (2) is changed to [16]:

Table 5 Enthalpies of dissolution of reactants and product of reaction (6) in the selected solvents ($T = 298.15 \pm 0.001$ K and $P = 101.22 \pm 0.01$ kPa)

System	Solvent	No.	W/g	$\Delta E_s/\Delta E_e$	t_e/s	Q_s/J	$\Delta_s H_m^o$ /kJ mol^{-1}
D-C$_6$H$_{10}$O$_6$(s)	s	1	0.17833	−1.0046	37.437	18.249	18.230
		2	0.17826	−0.9081	41.078	18.100	18.100
		3	0.17840	−0.9776	38.468	18.247	18.221
		4	0.17823	−0.9906	38.827	18.663	18.653
		5	0.17847	−0.8678	44.484	18.733	18.698
Avg. $\Delta_s H_{m,1}^o = (18.380 \pm 0.123)$ kJ mol^{-1}							
KOH(s)	Solution A$_1$	1	0.05700	1.3950	102.422	−69.328	−68.246
		2	0.05670	1.0295	138.390	−69.131	−68.412
		3	0.05691	1.3412	106.593	−69.371	−68.407
		4	0.05670	0.8750	162.859	−69.218	−68.498
		5	0.05673	1.5691	90.531	−68.927	−68.174
Avg. $\Delta_s H_{m,2}^o = -(68.347 \pm 0.059)$ kJ mol^{-1}							
K[D-C$_6$H$_{11}$O$_7$](s)	s	1	0.23405	−1.2379	39.172	23.530	23.551
		2	0.23425	−0.8759	46.016	23.058	23.040
		3	0.23430	−1.1480	40.922	22.795	22.790
		4	0.23443	−0.8795	54.250	23.152	23.134
		5	0.23435	−1.4125	33.390	22.886	22.876
Avg. $\Delta_s H_{m,3}^o = (23.078 \pm 0.133)$ kJ mol^{-1}							

In which $\Delta_s H_m^o = Q_s/n = -(\Delta E_s/\Delta E_e) \cdot I^2 R t_e (M/W)$, $\Delta_s H_m^o$ is standard molar enthalpy of dissolution of the sample, Q_s is heat effect of sample dissolution, n is the mole number of the sample, ΔE_s is the voltage change during the sample dissolution, ΔE_e is the voltage change during the electrical calibration, I is the electric current through the heater ($I = 20.00$ mA), R is the electrical resistance of the heater ($R = 1216.9$ Ω at $T = 298.15$ K), t_e is the heating duration of electrical calibration, M is the molar mass of the sample, and W is mass of sample. $\sigma_a = \sqrt{\sum_{i=1}^n (x - \bar{x})^2/n(n-1)}$, where $\bar{x}$ is the mean value of a set of measurement results, n is the experimental number, x_i is a single value in a set of measurements. "s": double-distilled water. For potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s): Solution A$_1$: {D-C$_6$H$_{10}$O$_6$(s)} + "s". Solution A: {KOH(s)} + Solution A$_1$. Solution B: {K[D-C$_6$H$_{11}$O$_7$](s)} + "s". After the reaction is complete, the final molalities of K[D-C$_6$H$_{11}$O$_7$](s) in solution A and solution B are the same, 1.0×10^{-2} mol kg^{-1}

$$U_{POT} = \gamma(\rho/M_m)^{1/3} + \delta \qquad (4)$$

where the values of the constants for MX (1:1) are: $\gamma = 1981.2$ kJ mol^{-1} cm and $\delta = 103.8$ kJ mol^{-1}. Lattice potential energy of the compound is determined to be $U_{POT}\{K[D-C_6H_{11}O_7]\} = 492.56$ kJ mol^{-1}, which reveals that the structure of K[D-C$_6$H$_{11}$O$_7$] is stable.

In addition, for a salt of molecular formula M_pX_q,

$$V_m(M_pX_q) = pV_+ + qV_- \qquad (5)$$

where V_- and V_+ are the volumes of the anion and cation, $p = 1$ and $q = 1$ for K[D-C$_6$H$_{11}$O$_7$]. $V_+(K^+)$ is 0.0277 nm^3 according to the literature [17], The V_- (the volume of the anion D-C$_6$H$_{11}$O$_7^-$) is estimated to be 0.1921 nm^3.

Standard molar enthalpy of formation of the compound K[D-C$_6$H$_{11}$O$_7$](s)

The title compound is supposed to be the product in the following chemical reaction. The designed reaction is shown in the following:

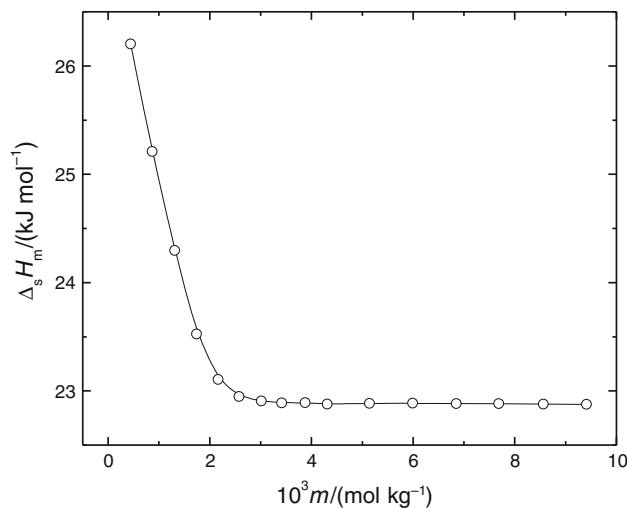$$D\text{-}C_6H_{10}O_6(s) + KOH(s) = K[D\text{-}C_6H_{11}O_7](s) \qquad (6)$$
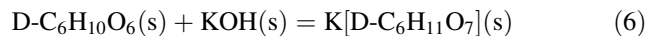
The standard molar enthalpies of dissolution of the reactants and product of the reaction (6) in the selected solvent (100 cm^3 of double-distilled water) are measured by an isoperibol solution–reaction calorimeter, respectively. The enthalpy change of the reaction is calculated from the data of above standard molar enthalpies of dissolution.

The samples KOH(s) and D-C$_6$H$_{10}$O$_6$(s) used in the solution calorimetry are of analytical grade and newly bought from J&K Scientific Ltd, China. Purity of D-C$_6$H$_{10}$O$_6$(s) is analyzed to be >99.5% by elemental analysis and HPLC. The labeled purity of the KOH(s) is more than 99.99% in mass percentage, when bought and delivered to our laboratory it is sealed in good condition in a small glass bottle. Weighing the sample KOH(s) used in the solution–reaction calorimetric experiments is carried out in the clean glove box containing the high-purity nitrogen, and a suitable cap made from polytetrafluoroethylene (PTFE) is

Table 6 Values of molar solution enthalpies of potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s) with different molalities ($T = 298.15 \pm 0.001$ K and $P = 101.22 \pm 0.01$ kPa)

$10^3 m$/mol kg^{-1}	$\Delta_s H_m$/kJ mol^{-1}	$-m$/mol kg^{-1}	$-my'$/mol kg^{-1}	$-0.5m^2$/mol^2 kg^{-2}	Y	$10^{-5}/(\partial^\Phi L/\partial m)_{T,P}$	$^\Phi L$/kJ mol^{-1}	$\overline{L}_1$/J mol^{-1}	$\overline{L}_2$/kJ mol^{-1}
0.444	26.20	−4.44E−4	−4.32E−4	−9.86E−08	0.01770	−30.650	−1.720	10.875	−1.363
0.866	25.21	−8.66E−4	−8.33E−4	−3.75E−07	0.01702	−21.592	−2.712	29.131	−1.872
1.311	24.30	−0.00131	−0.00125	−8.59E−07	0.01639	−15.321	−3.626	47.398	−2.012
1.742	23.52	−0.00174	−0.00165	−1.52E−06	0.01586	−10.941	−4.397	59.774	−1.911
2.163	23.11	−0.00216	−0.00203	−2.34E−06	0.01557	−7.700	−4.816	64.822	−1.670
2.574	22.95	−0.00257	−0.00241	−3.31E−06	0.01546	−5.234	−4.974	62.433	−1.352
3.012	22.91	−0.00301	−0.00280	−4.54E−06	0.01543	−3.198	−5.015	52.214	−0.968
3.416	22.89	−0.00342	−0.00316	−5.84E−06	0.01541	−1.742	−5.034	36.606	−0.600
3.877	22.89	−0.00388	−0.00357	−7.52E−06	0.01540	−0.4924	−5.031	13.326	−0.196
4.311	22.88	−0.00431	−0.00395	−9.29E−06	0.01539	0.3515	−5.045	−11.759	0.146
5.141	22.88	−0.00514	−0.00468	−1.32E−05	0.01539	1.236	−5.037	−58.808	0.630
5.989	22.89	−0.00599	−0.00541	−1.79E−05	0.01539	1.344	−5.036	−86.812	0.800
6.850	22.88	−0.00685	−0.00614	−2.35E−05	0.01537	0.8020	−5.040	−67.735	0.544
7.684	22.88	−0.00768	−0.00684	−2.95E−05	0.01537	−0.2367	−5.040	25.162	−0.187
8.561	22.88	−0.00856	−0.00757	−3.66E−05	0.01536	−1.785	−5.043	235.44	−1.533
9.411	22.88	−0.00941	−0.00828	−4.43E−05	0.01536	−3.663	−5.047	583.88	−3.452

In which m is the molality of the solute, $\Delta_s H_m$ is the molar enthalpy of dissolution of the compound, $y' = [1-(1 + 2I^{1/2})\exp(-2I^{1/2})]/2I$, and Y is the extrapolation function. $^\Phi L$ is the apparent relative molar enthalpy; $\overline{L}_1$ is the relative partial molar enthalpy of the double-distilled water; $\overline{L}_2$ is the relative partial molar enthalpy of the compound


Fig. 4 Plot of the measured $\Delta_s H_m$ against molality for potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s) at $T = 298.15$ K

covered to the sample cell because KOH(s) is a kind of the air sensitive and hygroscopic compound.

About 1.0×10^{-3} mol of D-C$_6$H$_{10}$O$_6$(s) in the reaction (6) is dissolved in 100 cm^3 of double-distilled water at $T = 298.15$ K. The experimental results of the process are shown in Table 5. If "s" represented 100 cm^3 of double-distilled water, the dissolution process may be expressed as:

$$\{\text{D-C}_6\text{H}_{10}\text{O}_6(s)\} + \text{``s''} = \text{Solution A}_1 \tag{7}$$

The stoichiometric number of KOH(s) $\{n(\text{D-C}_6\text{H}_{10}\text{O}_6(s)):n(\text{KOH(s)}) = 1:1\}$ in the reaction (6) is regarded as a norm for sample weighing, about 1.0×10^{-3} mol of KOH(s) is dissolved in the solution A$_1$ at $T = 298.15$ K. The experimental results of the process are shown in Table 5 and the dissolution process may be expressed as:

$$\{\text{KOH(s)}\} + \text{Solution A}_1 = \text{Solution A} \tag{8}$$
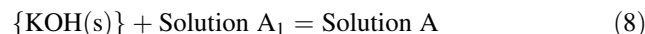
The enthalpies of dissolution of the product in 100 cm^3 of double-distilled water are measured under the same condition as the above. The experimental results of the process are listed in Table 5, and the dissolution process may be expressed as:

$$\{\text{K[D-C}_6\text{H}_{11}\text{O}_7](s)\} + \text{``s''} = \text{Solution B} \tag{9}$$
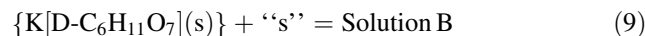
Then the enthalpy change of the reaction (6) can be calculated in accordance with the experimental results as follows:

$$
\begin{aligned}
\Delta_r H_m^o &= \sum \Delta_s H_m^o(\text{reactants}) - \sum \Delta_s H_m^o(\text{products}) \\
&= \Delta_s H_{m.1}^o + \Delta_s H_{m.2}^o - \Delta_s H_{m.3}^o \\
&= 18.380 - 68.347 - 23.078 \\
&= -(73.045 \pm 0.191) \text{ kJ mol}^{-1}.
\end{aligned}
$$

The enthalpy change of the reaction (6) is combined with some auxiliary thermodynamic data,

$\Delta_f H_m^o(C_6H_{10}O_6, s) = -1256.4$ kJ mol^{-1} [18] and $\Delta_f H_m^o(KOH, s) = -424.72$ kJ mol^{-1} [19], the standard molar enthalpy of formation of K[D-C$_6$H$_{11}$O$_7$](s) is determined to be:

$$
\begin{aligned}
\Delta_f H_m^o(C_6H_{11}O_7K, s) &= \Delta_r H_m^o + \Delta_f H_m^o(C_6H_{10}O_6, s) \\
&\quad + \Delta_f H_m^o(KOH, s) \\
&= -73.045 - 1256.4 - 424.72 \\
&= -(1754.17 \pm 0.19) \text{ kJ mol}^{-1}.
\end{aligned}
$$

The results of refractive indexes are the important information used to detect whether the difference of the structure and chemical composition between two solutions exists. We have measured the refractive indexes of the two solutions by Abbe refractometer. Uncertainty of the instrument is ±0.0003. The experimental temperature in the room is (20.0 ± 0.1) °C. In this paper, the measured values of the refractive indexes of solution A and solution B are (1.3309 ± 0.0002) and (1.3308 ± 0.0003) for the aqueous solution of K[D-C$_6$H$_{11}$O$_7$](s), respectively. The results indicate that solution A is consistent with solution B, and there is no difference in the structure, chemical components and physicochemical properties between the two solutions. Therefore, the designed thermochemical cycle is reasonable and reliable and can be used to calculate the standard molar enthalpy of formation of K[D-C$_6$H$_{11}$O$_7$](s).

Molar enthalpy of dissolution at infinite dilution and Pitzer's parameters

The title compound is soluble in the double-distilled water. The experimental values of molar enthalpies of dissolution $(\Delta_s H_m)$ of the title compound in the double-distilled water are given in Table 6, and the curvilinear relationship of $\Delta_s H_m/$(kJ mol^{-1}) with molalities $m/$(mol kg^{-1}) is shown in Fig. 4.

The molar enthalpy of dissolution of the compound $(\Delta_s H_m)$ in the double-distilled water is expressed as [20, 21]:

$$\Delta_s H_m = \Delta_s H_m^\infty + {}^\phi L \tag{10}$$

in which $\Delta_s H_m^\infty$ is the molar enthalpy of dissolution at infinite dilution, $^\Phi L$ is the apparent relative molar enthalpy. For the salt of MX (1:1), the apparent relative molar enthalpy $^\Phi L$ may be expressed as: [22]

$$
\begin{aligned}
{}^\Phi L = {}&\nu|z_M z_X| A_H \ln\left(1 + bI^{1/2}\right)/2b \\
&- 2\nu_M \nu_X RT^2 \left[m\beta_{MX}^{(0)L} + my'\beta_{MX}^{(1)L} + (\nu_M \nu_X)^{1/2} m^2 C_{MX}^{\Phi L}/2 \right]
\end{aligned}
\tag{11}
$$

where I is ionic strength ($\sum m_i z_i^2/2$), $\beta_{MX}^{(0)L}$, $\beta_{MX}^{(1)L}$, and $C_{MX}^{\Phi L}$ are Pitzer's parameters for enthalpy, the coefficients $\beta_{MX}^{(0)L}$ and $\beta_{MX}^{(1)L}$ account for various types of short-range interactions between M and X, and for indirect forces arising from the solvent, the third coefficient $C_{MX}^{\Phi L}$ represents for triple ion interactions and is important only at high concentrations or with strong triple ion interaction [20]. In this paper, $C_{MX}^{\Phi L}$ may not be overlooked for the aqueous solution of K[D-C$_6$H$_{11}$O$_7$](s) because formation and breaking of the six-membered chelate ring of the D-C$_6$H$_{11}$O$_7^-$ anion with K$^+$ cation are similar to the three-ion interaction and further hydrolyzation of the D-C$_6$H$_{11}$O$_7^-$ anion takes place at low concentrations because the D-gluconic acid is a weak acid similar to acetic acid. The hydrolyzation reaction of the D-C$_6$H$_{11}$O$_7^-$ anion will produce the hydroxide ion, and a model of the triple ion interaction will be formed by K$^+$, D-C$_6$H$_{11}$O$_7^-$ anion and OH$^-$. ν is the total number of ions formed from the salt ($\nu = \nu_M + \nu_X$). z_M and z_X are the respective charges on the cation and anion of the compound. b is a parameter with the value 1.2 kg$^{1/2}$ mol$^{-1/2}$ for all solutions. $y' = 2[1 - (1 + \alpha I^{1/2})\exp(-\alpha I^{1/2})]/\alpha^2 I$ and $\alpha = 2.0$ kg$^{1/2}$ mol$^{-1/2}$. $m/$(mol kg^{-1}) is the molality of the compound. R is molar gas constant, 8.3145 J mol^{-1} K^{-1}. A_H is Debye–Huckel parameter for enthalpy [20, 21], $A_H = 1986$ J mol^{-1} at $T = 298.150$ K.

For the case of salt of formula MX with charge ratio (1:1) such as K[D-C$_6$H$_{11}$O$_7$](s), the apparent relative molar enthalpy $^\Phi L$ for K[D-C$_6$H$_{11}$O$_7$](s) may be expressed as:

$$
\begin{aligned}
{}^\Phi L = {}&2(A_H/2.4)\ln\left(1 + 1.2I^{1/2}\right) \\
&- 2RT^2 \left[m\left(\beta_{MX}^{(0)L} + y'\beta_{MX}^{(1)L}\right) + m^2 C_{MX}^{\Phi L}/2 \right]
\end{aligned}
\tag{12}
$$
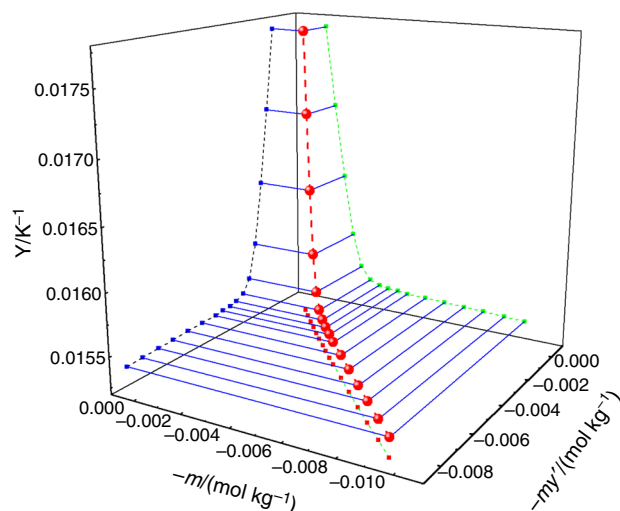
Fig. 5 The 3D chart of Y against $-m$ and $-my'$ for potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s)

From Eqs. (10) and (12), the working equation to determine Pitzer's parameters is shown as:

$$Y = \left[\Delta_s H_m - A_H \ln\left(1 + 1.2 I^{1/2}\right)/1.2\right]/(2RT^2)$$
$$= \alpha_0 - m\beta_{MX}^{(0)L} - my'\beta_{MX}^{(1)L} - m^2 C_{MX}^{\Phi L}/2 \quad (13)$$

where Y is the extrapolation function and $\alpha_0 = \Delta_s H_m^\infty/(2RT^2)$. Regression of Y against $-m$, $-my'$ and $-0.5\ m^2$ is made by least squares to obtain $\alpha_0 = 0.01889$, $\beta_{MX}^{(0)L} = -51.9832$, $\beta_{MX}^{(1)L} = 56.1199$ and $C_{MX}^{\Phi L} = 639.1015$ with a standard deviation of the fitting 1.45278×10^{-4} for K[D-C$_6$H$_{11}$O$_7$](s), respectively. The molar enthalpy of dissolution for the title compound at infinite dilution is determined to be $\Delta_s H_{m\{K-D-C_6H_{11}O_7](s)\}}^\infty = (27.92 \pm 0.21)$ kJ mol^{-1}. The 3D chart of Y against $-m$ and $-my'$ is plotted in Fig. 5.

The quantities $\beta_{MX}^{(0)L}$ and $\beta_{MX}^{(1)L}$ are attributed to the short-range interaction between the cation and anion. Generally speaking, the absolute values of $\beta_{MX}^{(0)L}$ and $\beta_{MX}^{(1)L}$ are very small for an usual electrolyte and have a tendency to increase along with the volume and the quantity of the ion. It may be noted that the absolute values of $\beta_{MX}^{(0)L}$ and $\beta_{MX}^{(1)L}$ are significantly greater than those of usual electrolytes mainly since the volume of the anion D-C$_6$H$_{11}$O$_7^-$ is greater than those of the usual electrolytes. This shows that various types of strong short-range interactions exist between cation and anion in the solutions obtained from dissolution of the title compound. $\beta_{MX}^{(0)L}$ is a negative value, that is, $\left(\partial\beta_{MX}^{(0)}/\partial T\right)_p < 0$, which indicates that the value of $\beta_{MX}^{(0)L}$ drops with the rise of the temperature. This shows that the interionic repulsive force decreases with the increase of the temperature. The third coefficient $C_{MX}^{\Phi L}$ for triple ion interactions has a very high value in the research, it may be ascribed to the chelate behavior of the D-C$_6$H$_{11}$O$_7^-$ anion with K$^+$ cation in the aqueous solution and further hydrolyzation of the D-C$_6$H$_{11}$O$_7^-$ anion at low concentrations, and the larger ionization energy of the electrovalent compound in water is caused mainly by the formation and destruction of the six-membered chelate ring and further hydrolyzation of the D-C$_6$H$_{11}$O$_7^-$ anion at low concentrations. The two processes need to absorb larger heat quantity than normal process.

The degree of chaos of K[D-C$_6$H$_{11}$O$_7$](s) is increased when it is dissociated to K$^+$(aq) and D-C$_6$H$_{11}$O$_7^-$(aq) in the double-distilled water. It is concluded that the entropy change of the dissolution reaction is greater than zero according to the statistical explanation of the entropy in statistical thermodynamics. From the values of molar enthalpies of dissolution, we deduce the conclusion that the dissolution of the title compound in the water is a typical endothermic process, and an entropy-driven process instead of enthalpy-driven process. It mainly ascribes to the breaking of ionic bonds, chelate bonds and van der Waals interaction forces existing in the compound needing to absorb large amount of heat energy.

Relative partial molar enthalpies

The relative partial molar enthalpies of solvent ($\overline{L_1}$) and solute ($\overline{L_2}$) are important thermodynamic functions of the electrolyte solution. Generally, there are many ways used to determine the relative partial molar enthalpies. In this paper, they are obtained by the apparent relative molar enthalpy ($^\Phi L$) and partial derivative of $^\Phi L$ against m.

The relative partial molar enthalpy of the double-distilled water ($\overline{L_1}$) as the solvent is expressed as:

$$\bar{L}_1 = -M_{H_2O} m^2 \left(\partial^\Phi L/\partial m\right)_{T,P} \quad (14)$$

The formula to determine relative partial molar enthalpy of the each compound ($\overline{L_2}$) is,

$$\bar{L}_2 = {}^\Phi L + m\left(\partial^\Phi L/\partial m\right)_{T,P} \quad (15)$$

The partial derivative of $^\Phi L$ against m, $(\partial^\Phi L/\partial m)_{T,P}$, is obtained under constant pressure and temperature ($C_{MX}^{\Phi L}$ is not neglected):

$$\left(\partial^\Phi L/\partial m\right)_{T,P} = A_H/\left(2m^{1/2} + 2.4m\right)$$
$$- 2RT^2\left[\beta_{MX}^{(0)L} + \beta_{MX}^{(1)L}\exp\left(-2m^{1/2}\right) + mC_{MX}^{\Phi L}\right] \quad (16)$$

According to the relationships shown in Eqs. (10), (14), (15), and (16), apparent relative molar enthalpies ($^\Phi L$) and relative partial molar enthalpies of the double-distilled water ($\overline{L_1}$) as the solvent and the title compounds ($\overline{L_2}$) as the solute are obtained. All the results calculated above are listed in Table 6.

Standard molar enthalpy of formation of the anion [D-C$_6$H$_{11}$O$_7$]$^-$(aq) in the aqueous solution

The potassium D-gluconate K[D-C$_6$H$_{11}$O$_7$](s) is dissociated into the anion [D-C$_6$H$_{11}$O$_7$]$^-$ and the cation K$^+$ in the aqueous solution according to the following ionization equation,

$$K[D\text{-}C_6H_{11}O_7](s) \rightarrow K^+(aq) + [D\text{-}C_6H_{11}O_7]^-(aq) \quad (17)$$
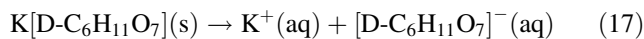
The standard molar enthalpy of formation of the anion [D-C$_6$H$_{11}$O$_7$]$^-$ in the aqueous solution is calculated according to Eq. 18 based on Eq. 17,

$$\Delta_f H_m^o\left(D\text{-}C_6H_{11}O_7^-, aq\right) = \Delta_{sol}H_m^\infty$$
$$+ \Delta_f H_m^o(K[D\text{-}C_6H_{11}O_7],s) - \Delta_f H_m^o(K^+,aq) \quad (18)$$

The standard molar enthalpy of formation of the anion [D-$C_6H_{11}O_7]^-$(aq) is calculated to be $\Delta_f H_m^o$ $(D\text{-}C_6H_{11}O_7^-, aq) = -(1473.87 \pm 0.28)$ kJ mol^{-1} through the molar enthalpy of dissolution at infinite dilution $\Delta_{sol}H_m^\infty = (27.92 \pm 0.21)$ kJ mol^{-1} and some auxiliary thermodynamic data, such as $\Delta_f H_m^o(K^+, aq) = -252.38$ kJ mol^{-1} [20], and $\Delta_f H_m^o(K[D\text{-}C_6H_{11}O_7], s) = -(1754.17 \pm 0.19)$ kJ mol^{-1}, as described in the paper.

Conclusions

1. Potassium D-gluconate $K[D\text{-}C_6H_{11}O_7]$(s) is synthesized, and the crystal structure is determined by X-ray crystallography. The lattice potential energy is determined to be $U_{POT}[K[D\text{-}C_6H_{11}O_7]] = 492.56$ kJ mol^{-1}. The ionic volume of $D\text{-}C_6H_{11}O_7^-$ is calculated to be 0.1921 nm^3.

2. In accordance with Hess' law, reasonable thermochemical cycle is designed, and the standard molar enthalpy of formation of potassium D-gluconate $K[D\text{-}C_6H_{11}O_7]$(s) is calculated to be $-(1754.17 \pm 0.19)$ kJ mol^{-1}.

3. The molar enthalpy of dissolution of the compound at infinite dilution is calculated to be (27.92 ± 0.21) kJ mol^{-1}. The standard molar enthalpy of formation of the anion [D-$C_6H_{11}O_7]^-$(aq) is calculated to be $\Delta_f H_m^o(D\text{-}C_6H_{11}O_7^-, aq) = -(1473.87 \pm 0.28)$ kJ mol^{-1}. The Pitzer's parameters ($\beta_{MX}^{(0)L}$, $\beta_{MX}^{(1)L}$ and $C_{MX}^{\Phi L}$) are obtained through Pitzer's theory.

4. The values of apparent relative molar enthalpies ($^\Phi L$) and relative partial molar enthalpies of the solvent ($\overline{L_1}$) and the compounds ($\overline{L_2}$) are derived, respectively.

Supplementary material

CCDC 888208 for $K[D\text{-}C_6H_{11}O_7]$(s) contains the supplementary crystallographic data for the title compound. The data can be obtained free of charge via http://www.ccdc.cam.ac.uk/deposit or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk.

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