Short communication

A new lithium salt with tetrafluoro-1,2-benzenediolato and lithium tetrafluoroborate for lithium battery electrolytes

Zhao-Ming Xue [a,*], Xiao-Fen Zhang [a], Wei Zhou [a], Chun-Hua Chen [b]

[a] Department of Chemistry, Anhui University, Hefei, Anhui 230039, PR China
[b] Department of Materials Science and Engineering, University of Science and Technology of China, Hefei, Anhui 230026, PR China

ABSTRACT

A new unsymmetrical lithium salt containing F^-, $C_6O_2F_4^{2-}$ [dianion of tetrafluoro-1,2-benzenediol], lithium difluoro[tetrafluoro-1,2-benzenediolato(2-)-O,O′]borate (4FLDFBDB) is synthesized and characterized. The thermal characteristics of it, and its derivatives, lithium difluoro[3-fluoro-1,2-benzenediolato(2-)-O,O′]borate (FLDFBDB), and lithium difluoro[1,2-benzene-diolato(2-)-O,O′]borate (LDFBDB) are examined by thermogravimetric analysis (TG). The thermal decomposition in air begins at 170 °C, 185 °C, and 230 °C for 4FLDFBDB, FLDFBDB, and LDFBDB respectively. The order of the stability toward oxidation of these organoborates is 4FLDFBDB > FLDFBDB > LDFBDB. The cyclic voltammetry study shows that the 4FLDFBDB solution in propylene carbonate (PC) is stable up to 4.2 V versus Li^+/Li. They are soluble in common organic solvents. Ionic dissociation properties of 4FLDFBDB and its derivatives are examined by conductivity measurements in PC, PC + ethyl methyl carbonate (EMC), PC + dimethyl ether (DME), PC + ethylene carbonate (EC) + EMC. The conductivity values of the 0.10 mol dm^{-3} 4FLDFBDB electrolyte in these solutions are higher than those of FLDFBDB and LDFBDB electrolytes.

© 2011 Elsevier B.V. All rights reserved.

1. Introduction

Many researchers have attempted to develop improved electrolytes for lithium batteries with high energy density and long cycle life [1–3] as power sources for portable electronic instruments and electric vehicles in order to protect the environment and natural resources. Barthel et al. reported a new class of electrochemically and thermally stable lithium salts [4,5] with a chelate-type boron-containing anion, such as bis[tetrafluoro-1,2-benzenediolato(2-)-O,O′]borate(4FLBBB) [6]. Xu et al. also reported lithium bis(oxalate) borate (LBOB) and lithium [malonato oxalato]borate (LMOB) as advanced electrolytes for Li-ion battery [7,8]. Recently, a novel lithium salt, lithium oxalyldifluoroborate (LODFB) [9], has drawn intensive attention because of its significant merit such as (1) the ability to support metallic lithium cycling reversibly on the surface of copper anode current collector, (2) the ability to passivate aluminum cathode current collector at high potentials, (3) the ability to participate in formation of the SEI and support Li-ion battery operating stably at high temperatures, and (4) the ability to increase battery safety protection and overcharge tolerance [9–12]. The common feature of these anions is that extensive charge delocalization is present in them because they are composed of strongly electron-withdrawing substituents. Thus, the lithium salts of these anions yield sufficiently high ionic conductivity in solutions, which exhibit wide electrochemical stability windows and good thermal stability.

Based on our previous theoretical studies [13–18], anions with pronounced charge delocalization, F^- and $C_6O_2F_4^{2-}$ [dianion of tetrafluoro-1,2-benzenediol], are chosen as the unsymmetrical chelators to coordinate with boron to form lithium salt in this study to further our understanding on the relationship between the property and structure of these lithium salts. A new lithium salt, lithium difluoro[tetrafluoro-1,2-benzenediolato(2-)-O,O′]borate (4FLDFBDB), as shown in Fig. 1, was synthesized. Its thermal and electrochemical stabilities, conductivities in some solvent mixtures were studied and compared with those in the lithium difluoro[3-fluoro-1,2-benzene-diolato(2-)-O,O′]borate (FLDFBDB) and lithium difluoro[1,2-benzene-diolato(2-)-O,O′]borate (LDF-BDB) electrolytes.

To understand the properties of this new lithium salt at a quantum chemistry level, the density functional theory (DFT) B3LYP method was chosen. We will address the relationship between molecular structures and properties regarding the 4FDFBDB$^-$, FDFBDB$^-$, and DFBDB$^-$ anions and their lithium salts.

* Corresponding author. Tel.: +86 551 3861055; fax: +86 551 3861338.
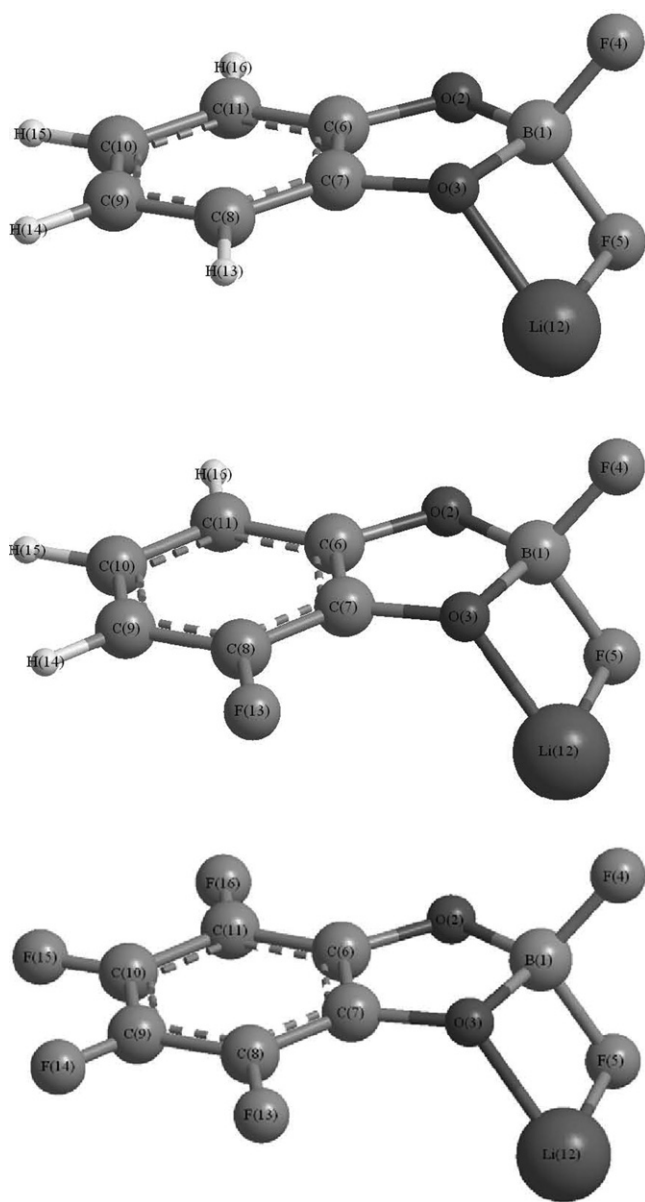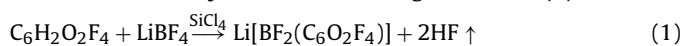E-mail address: zmxue@ahu.edu.cn (Z.-M. Xue).

Fig. 1. Structures of 4FLDFBDB, FLDFBDB and LDFBDB.

2. Experimental and computational methods

2.1. Synthesis

3,4,5,6-Tetrafluoro-1,2-benzenediol was synthesized according to the procedures given in Ref. [6].

4FLDFBDB was synthesized according to reaction (1):

$$C_6H_2O_2F_4 + LiBF_4 \xrightarrow{SiCl_4} Li[BF_2(C_6O_2F_4)] + 2HF \uparrow \qquad (1)$$

Specifically, in an argon-filled glove box, 0.01 mol $LiBF_4$, 0.01 mol tetrafluoro-1,2-benzenediol and 20 mL dimethyl carbonate (DMC) solvent were placed in a flask. SiCl4 was added drop-wise to the solution, which was then stirred overnight under purified nitrogen. The completion of the reaction was judged by making sure that gas generation stopped completely. Then, the solution was refluxed for 2 h at 50 °C under purified nitrogen until it becomes transparent. After that, the solvent DMC was evaporated on a rotary evaporator to obtain a solid product. It was purified by multi-time recrystallizations by dissolving into DMC and drying in vacuum at 60 °C for 2 h followed by 120 °C for 48 h. Then, the product was transferred

into the glove box. The yield for the purified salt was up to 90.05%. The purity of the compound was examined by inductively coupled plasma (ICP, Poasma–Spec) analysis for Li and B contents. The ^{1}H NMR and ^{13}C NMR spectroscopy (DMX-500, Bruker) of the prepared solid in dimethyl sulfoxide (DMSO-d_6) was also performed.

Meanwhile, FLDFBDB and LDFBDB were synthesized with the procedures described previously [17,18]. The purification procedures for propylene carbonate (PC), ethylene carbonate (EC), 1,2-dimethoxyethane (DME), ethyl methyl carbonate (EMC), were the same as given in Barthel et al.'s paper [6].

Excess amounts of solid compound (4FLDFBDB, FLDFBDB and LDFBDB) are placed into 5 mL vials containing solvent (PC, PC + EMC, PC + DME, PC + EC + EMC). The vials are sealed and placed into a glove box at 25 °C for 6 days, and stirred for a while each 12 h until equilibrium is evident. The upper clear solution is taken for measuring solubility by ICP analysis for Li and B contents.

Thermogravimetric analyses (TGA) of the 4FLDFBDB, FLDFBDB, LDFBDB were carried out with Perkin–Elmer Pyres-1 DMDA-V1 model, using a sample of about 10 mg. The decomposition voltages (i–E curves) of the electrolytes using a three-electrode system (platinum wire with a surface area of 4.91×10^{-4} cm^2 as working electrode, and Li plate as both counter and reference electrodes) were measured at a scan rate of 9 mV s^{-1}. The preparation of the electrolyte solutions and the cell assembly were carried out in a glove box (Labmaster 130, MBRAUN) at low water (<1 ppm), and oxygen (<1 ppm) contents.

2.2. Computation

The local minima of the complexes have been fully optimized by analytic gradient techniques. The method used was the density functional theory (DFT) with Becke's three parameters (B3) exchange functional along with the Lee–Yang–Parr (LYP) non-local correlation functional (B3LYP). All of the complexes were treated with DFT method at B3LYP/6-31++G(2df,2p) level for full geometry optimization. Nature population analysis (NPA) and natural bond orbital (NBO) [19] analysis were performed at B3LYP/6-311++G(3df,3pd) level using NBO program to obtain quantitative analysis of cation-anion interactions between NBOs of the complexes.

Single-point energy calculations were performed to obtain more accurate energies at higher level basis set (B3LYP/6-311++G(3df, 3pd)//B3LYP/6-31++G(2df,2p)). The HF method at the same level computation was performed for comparing with DFT at some cases. All of the HF, DFT and NBO calculations were performed using the Gaussian 03 program package [20].

3. Results and discussion

3.1. The composition and structure of 4FLDFBDB

The ICP analysis of the synthesized solid contains Li 2.90% and B 4.65%. These data are close to the calculated values Li 2.94% and B 4.58% for 4FLDFBDB, meaning that a pure 4FLDFBDB product has been successfully obtained. ^{13}C NMR spectrum of this product (not shown here) gives three signals at chemical shifts of 137.17 (C6/C7), 135.40 (C8/C11), 132.91 (C9/C10) ppm. It can be concluded from the ICP and the NMR spectra that fairly pure crystallization product (shown in Fig. 1) have been obtained in this work.

3.2. Thermal stability

Fig. 2 shows the TG curves of the lithium organoborates in N$_2$. It can be seen that the salt decomposition starts to occur at 170, 185, and 230 °C for LDFBDB, FLDFBDB, and 4FLDFBDB, respectively.
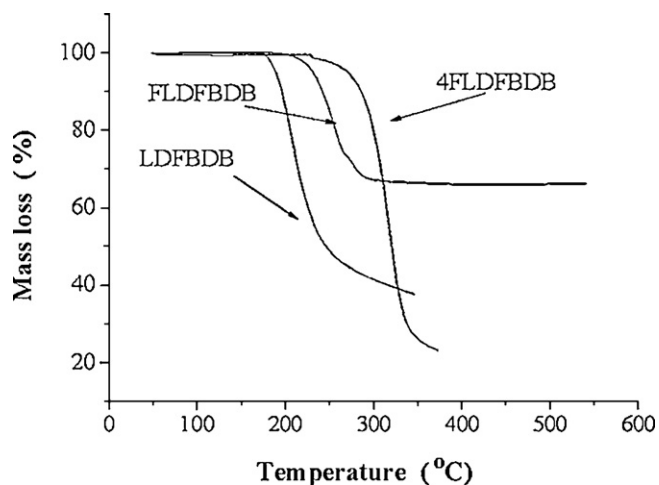
Fig. 2. TG Curves of lithium organoborates at heating rate of $10\,^{\circ}C\,min^{-1}$ in N_2. α-Alumina was used as a reference.

Table 1
Solubility (S, $mol\,dm^{-3}$) of lithium salts in PC, PC-based equimolar binary solutions at 25 °C.

	PC (S, $mol\,dm^{-3}$)	PC + DME (S, $mol\,dm^{-3}$)	PC + EMC (S, $mol\,dm^{-3}$)	PC + EC + EMC (S, $mol\,dm^{-3}$)
LDFBDB	0.518	0.564	0.592	0.619
FLDFBDB	0.443	0.464	0.501	0.522
4FLDFBDB	0.306	0.265	0.286	0.318

Therefore, among the three salts 4FLDFBDB exhibits a thermal stability higher than those of FLDFBDB and LDFBDB. Furthermore, it seems that the thermal stability depends on the higher conjugate energies of the chelate-type anion with boron [21].

3.3. Solubility

Similar to LDFBDB and FLDFBDB, 4FLDFBDB is stable in organic electrolyte solutions but it may be decomposed by hydrolysis in aqueous solutions and converted to HF, $C_6H_2O_2F_4$, and H_3BO_3. They are moderately soluble in PC + EC + EMC with a solubility of $0.318\,mol\,dm^{-3}$ at 25 °C for 4FLDFBDB (Table 1). The solubilities of the lithium salts in PC + EC + EMC are some greater than those in PC, and PC-based equimolar binary solutions.

As can be seen in Table 2, the solubility of 4FLDFBDB salt is the smallest among the three salts in PC solutions. According to our previous theoretical researches [13], we have also chosen to calculate a theoretical set of parameters of TLSER (theoretical linear solvation energy relationships), developed by Cramer et al. [22], and correlated them with the solubility of a lithium salt.

The equation [22] has been applied to the three anions (DFBDB$^-$, FDFBDB$^-$, and 4FDFBDB$^-$). With B3LYP/6-311++G(3df,3pd)//B3LYP/6-31++G(2df,2p)-derived descriptors (Table 2), We obtain a result that the solubility, S, of a lithium salt to be most sensitive to anion polarizability π^*. The regression is of

$$\text{Log}(S) = -8.9295 + 0.0864\pi* \quad (R = 0.9999, \text{SD} = 0.0024)$$

Table 2
Solubility (S, $mol\,dm^{-3}$), descriptors of anions at B3LYP/6-311++G(3df,3pd) level, and corresponding conductivity (σ, $mS\,cm^{-1}$) of lithium salts in PC solutions at 25 °C.

	DFBDB$^-$	FDFBDB$^-$	4FDFBDB$^-$
S (m, PC, 298.2k)	0.518	0.443	0.306
Log(S)	−0.285	−0.354	−0.514
π^* (a.u.)	100.0	99.24	97.36
σ ($mS\,cm^{-1}$)	1.18	1.88	2.80

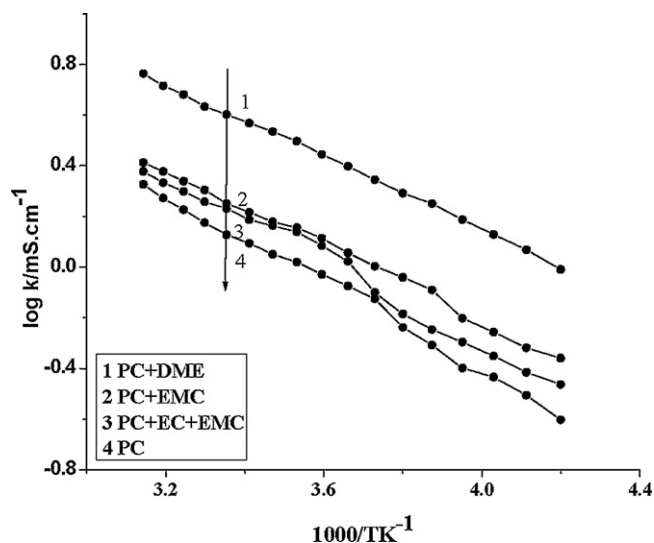**Fig. 3.** Temperature dependence of ionic conductivities of 4FLDFBDB solutions ($0.10\,mol\,dm^{-3}$) in different solvents.

3.4. Conductivity

Fig. 3 shows the temperature dependence of ionic conductivity of $0.10\,mol\,dm^{-3}$ 4FLDFBDB in PC solvent. We also include data for solutions in the mixed solvents of PC + DME, PC + EMC and PC + EC + EMC (mass ratio 1:1 and 1:1:1). A $0.10\,mol\,dm^{-3}$ solution of 4FLDFBDB in PC shows a conductivity of $1.34\,mS\,cm^{-1}$ at 25 °C. The solution of $0.10\,mol\,dm^{-3}$ 4FLDFBDB in PC–DME has room temperature conductivity of as high as $4.81\,mS\,cm^{-1}$, indicating that the ions in 4FLDFBDB solutions are highly disassociated. As can be seen in Fig. 3, the conductivity of the $0.10\,mol\,dm^{-3}$ 4FLDFBDB electrolyte solution in PC–DME is greater than those in the other solvents. Apparently, 4FLDFBDB is highly dissociating in PC–DME mixture.

Table 3 compares the conductivities of $0.10\,mol\,dm^{-3}$ 4FLDF-BDB solutions in different solvents with those of FLDFBDB and LDFBDB. It is clear that 4FLDFBDB solutions with the same concentration show conductivities higher than those of FLDFBDB and LDFBDB solutions. On the other hand, for the saturated solutions of each lithium salt in the solvent of PC, which concentrations are $0.306\,mol\,dm^{-3}$ for 4FLDFBDB, $0.443\,mol\,dm^{-3}$ for FLDFBDB and $0.518\,mol\,dm^{-3}$ for LDFBDB, they all have a quite high conductivity, 2.80, 1.88, and $1.18\,mS\,cm^{-1}$ for 4FLDFBDB, FLDFBDB and LDFBDB, respectively.

The disassociation of a lithium salt in the electrolyte solution is one of the key elements affecting Li-ion battery performance. It determines the number of free ions in an electrolyte, and thus the electric conductivity. Ue and Mori analyzed the contribution of the number of ions and the ion mobility to the electric conductivity for a variety of Li-ion nonaqueous electrolytes [23]. They found that the contribution from the number of free ions is generally larger

Table 3
Specific conductivities in different solvents containing $0.10\,mol\,dm^{-3}$ lithium organoborates at 25 °C.

Organoborate	Specific conductivity ($mS\,cm^{-1}$)			
	PC	PC + EMC (1:1)	PC + DME (1:1)	PC + EC + EMC (1:1:1)
LDFBDB	0.414	1.124	2.167	0.960
FLDFBDB	1.06	1.24	3.46	1.18
4FLDFBDB	1.341	1.78	4.81	1.70

Table 4
NBO energetic analysis for LDFBDB, FLDFBDB, and 4FLDFBDB at B3LYP/6-311++G(3df,3pd) level (energies in kJ mol^{-1}).
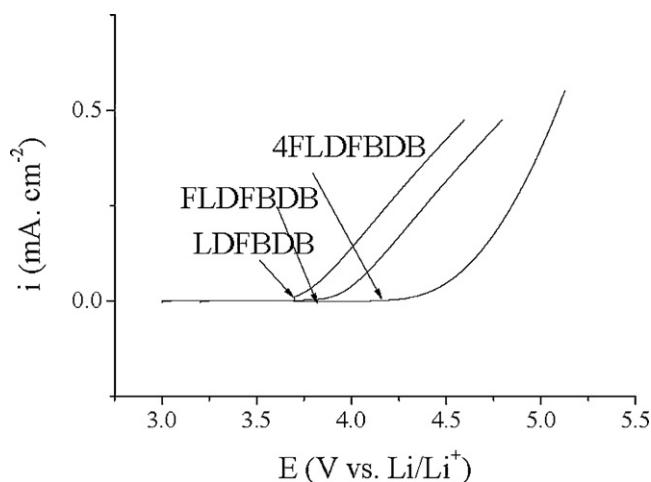
	LDFBDB	FLDFBDB	4FLDFBDB
$n^1_{O1} \rightarrow n^*_M$	4.46	4.24	4.09
$n^2_{O1} \rightarrow n^*_M$	1.15	1.07	1.07
$n^1_{F2} \rightarrow n^*_M$	3.20	3.06	2.98
$n^2_{F2} \rightarrow n^*_M$	0.56	0.54	0.49
$n^3_{F2} \rightarrow n^*_M$	2.20	2.06	1.89
$n^4_{F2} \rightarrow n^*_M$	0.62	0.54	–
E_{int}	12.19	11.51	10.52

Table 5
Limiting oxidation potentials, ionization potential calculations using DFT methods at 6-311++G(3df,3pd) level.

Anion	DFBDB$^-$	FDFBDB$^-$	4FDFBDB$^-$
$E_{radical}$ (a.u.)	−606.398611	−705.663842	−1003.449936
E_{anion} (a.u.)	−606.532456	−705.806818	−1003.611256
ΔE (kJ mol^{-1})	351.41	375.38	423.54
$ZPE_{radical}$ (kJ mol^{-1})	0.097174	0.088813	0.064237
ZPE_{anion} (kJ mol^{-1})	0.096576	0.088500	0.064281
ΔZPE (kJ mol^{-1})	−1.57	−0.82	0.12
I_p (eV)	3.66	3.90	4.39
E_{ox} (V vs. Li$^+$/Li)	3.7	3.9	4.2

than that from the ion mobility. Thus, the number of ions available plays a major role in determining the electric conductivity of a cell, and hence in the overall battery performance.

As generally recognized, the weaker the coordinating, the easier the separating of an ion-pair is. Natural bond orbital (NBO) analysis is carried out to further our understanding of orbital interactions and charge delocalization. Of particular interests are the interactions between O(F) (bounded with lithium cation) lone pairs and antibonding orbitals of lithium cation lone pair. The magnitudes of the interactions are shown in Table 4. With the increase of the number of F, it is interesting to notice that the calculated order of main orbital interaction energies (E_{int}) is E_{int}(LDFBDB) > E_{int}(FLDFBDB) > E_{int}(4FLDFBDB), although E_{int} only accounts for part of E_{bind}. In fact, E_{int} may be roughly attributed to the covalency contributions to binding. Thus, the electron transfer from anion (DFBDB$^-$, FDFBDB$^-$, 4FDFBDB$^-$) to Li$^+$ becomes lesser according to NPA and the effective cation charge becomes larger (+0.96694, +0.96825 and +0.96925 e for LDFBDB, FLDFBDB and 4FLDFBDB, respectively). Therefore, 4FDFBDB$^-$ is the weakest anion of the three salts and Li$^+$4FDFBDB$^-$ would be disassociated more than the other two salts at the same concentration of electrolyte solutions. Compared with the calculated data, the experimental conductivity (Table 3) increases with the effective cation charge, and decreases with E_{int} and the extent of electron transfer from anion to cation.

3.5. Electrochemical stability

The electrochemical stabilities of LDFBDB, FLDFBDB, and 4FLDFBDB solutions in PC on platinum wire electrode are shown in Fig. 4. The electrochemical oxidation potential can be obtained as ca. 4.2 V vs. Li$^+$/Li for the saturated solution of 4FLDFBDB in PC. This is higher than the oxidation potential for FLDFBDB–PC solution (3.9 V)
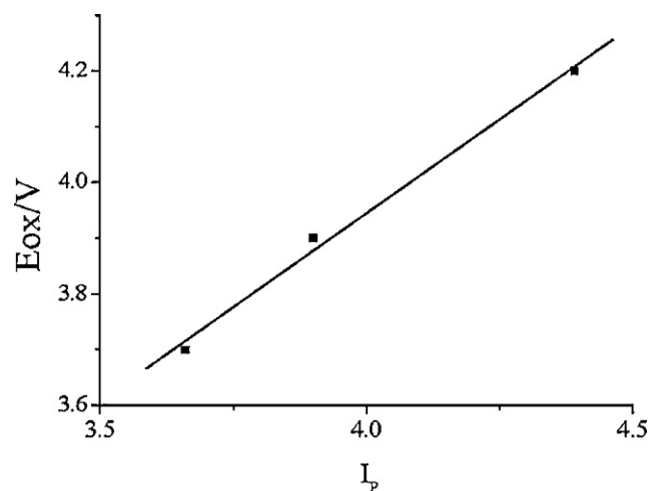

Fig. 5. Relation between E_{ox} and I_p of anions at DFT B3LYP/6-311++G (3df,3pd) level.

[17]. The order of the oxidation stability in these organoborates is 4FLDFBDB > FLDFBDB > LDFBDB.

Several studies of anion oxidation potentials were recently updated and extended by Xue et al. [24]. They have found that E_{ox} can be correlated with adiabatic ionization potential (I_p).

To further examine this experimental result, the ionization potentials were also calculated by *ab initio* density functional theory. This method usually gives higher accuracy in energy calculations, where the relative accuracies of various different model chemistries were considered by their performances on the G2 molecule sets [25]. The structural optimization of the anion was carried out by B3LYP/6-311++G(2df,2p) followed by the energy calculations on higher basis sets, 6-311++G(3df,3pd). The adiabatic ionization potential I_p was calculated from the energy difference ΔE between the total energy of the anion E_{anion} and that of the neutral radical $E_{radical}$ generated by one-electron oxidation. The structure and energy of the neutral radical was calculated by the same methods. Zero-point energies (ZPE) were also calculated by frequency analysis using B3LYP/6-31++G(2df,2p). The ionization potentials were calculated from the following equation

$$I_p = \Delta E - \Delta ZPE$$

The results are summarized in Table 5 and Fig. 5. Fig. 5 shows good correlation between I_p and E_{ox}, completely confirming the experimental result: E_{ox}(DFBDB$^-$) < E_{ox}(FDFBDB$^-$) < E_{ox}(4FDFBDB$^-$). The regression result is

$$E_{ox} = 1.24772 + 0.67421 \times I_p \quad (R = 0.99678, \quad SD = 0.02853)$$

4. Conclusions

A new lithium salt, lithium difluoro[tetrafluoro-1,2-benzenediolato(2-)-O,O′]borate (4FLDFBDB), with asymmetric

Fig. 4. *i–E* curves in PC saturated solutions using a platinum wire working electrode at a scan rate of 9 mV s^{-1} 20 °C.

chelatoborate anion, has been synthesized. The salt, 4FLDFBDB, is thermally stable and soluble in many of the common organic solvents used in batteries. The solutions are highly conductive and stable. The conductivities of 4FLDFBDB solutions are higher than those of FLDFBDB solutions. Its electrochemical oxidation potential is higher than that of FLDFBDB in the common organic solvents used in batteries. A strong correlation between the adiabatic ionization potential and the electrochemical stability is established. This proves that an extensive charge delocalization, in their anions, caused by strongly electron withdrawing anions (e.g. F^- and dianion of tetrafluoro-1,2-benzenediol) would raise the adiabatic ionization potential I_p, and improve the electrochemical stability of the electrolyte.

Acknowledgments

References

[1] N. Nanbu, K. Tsuchiya, T. Shibazaki, Y. Sasaki, Electrochem. Solid-State Lett. 5 (9) (2002) A202.
[2] M. Handa, M. Suzuki, J. Suzuki, H. Kanematsu, Y. Sasaki, Electrochem. Solid-State Lett. 2 (2) (1999) 60.
[3] X.M. Wang, E. Yasukawa, S. Kasuya, J. Electrochem. Soc. 147 (7) (2000) 2421.
[4] J. Barthel, A. Schmid, H.J. Gores, J. Electrochem. Soc. 147 (1) (2000) 21.
[5] J. Barthel, R. Buestrich, H.J. Gores, M. Schmidt, M. Wühr, J. Electrochem. Soc. 144 (1997) 3866.
[6] J. Barthel, R. Buestrich, E. Carl, H.J. Gores, J. Electrochem. Soc. 143 (11) (1996) 3572.
[7] W. Xu, C.A. Angell, Electrochem. Solid-State Lett. 4 (1) (2001) E1.
[8] W. Xu, A.J. Shusterman, R. Marzke, C.A. Angell, J. Electrochem. Soc. 151 (4) (2004) A632.
[9] S.S. Zhang, Electrochem. Commun. 8 (2006) 1423.
[10] K. Xu, S.S. Zhang, B.A. Poese, T.R. Jow, Electrochem. Solid-State Lett. 5 (2002) A259.
[11] K. Xu, S.S. Zhang, T.R. Jow, Electrochem. Solid-State Lett. 6 (2003) A117.
[12] G.V. Zhuang, K. Xu, T.R. Jow, P.N.J. Ross, Electrochem. Solid-State Lett. 7 (2004) A224.
[13] Z.M. Xue, C.H. Chen, Electrochim. Acta 49 (2004) 5167.
[14] Z.M. Xue, C.H. Chen, Prog. Chem. 17 (3) (2005) 399 (Chinese).
[15] Z.M. Xue, B. Liu, C.H. Chen, Electrochim. Acta 51 (2006) 4554.
[16] Z.M. Xue, C.Q. Ji, W. Zhou, C.H. Chen, J. Power Sources 195 (2010) 3689.
[17] Z.M. Xue, B.H. Zhao, C.H. Chen, J. Power Sources 196 (2011) 6478.
[18] Z.M. Xue, B.B. Sun, W. Zhou, C.H. Chen, J. Power Sources 196 (2011) 8710.
[19] E.D. Glendening, A.E. Reed, J.E. Carpenter, F. Weinhold, NBO Version 3.1.
[20] M.J. Frisch, G.W. Trucks, H.B. Schlegel, G.E. Scuseria, M.A. Robb, J.R. Cheeseman, J.A. Montgomery, T. Vreven Jr., K.N. Kudin, J.C. Burant, J.M. Millam, S.S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G.A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J.E. Knox, H.P. Hratchian, J.B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R.E. Stratmann, O. Yazyev, A.J. Austin, R. Cammi, C. Pomelli, J.W. Ochterski, P.Y. Ayala, K. Morokuma, G.A. Voth, P. Salvador, J.J. Dannenberg, V.G. Zakrzewski, S. Dapprich, A.D. Daniels, M.C. Strain, O. Farkas, D.K. Malick, A.D. Rabuck, K. Raghavachari, J.B. Foresman, J.V. Ortiz, Q. Cui, A.G. Baboul, S. Clifford, J. Cioslowski, B.B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R.L. Martin, D.J. Fox, T. Keith, M.A. Al-Laham, C.Y. Peng, A. Nanayakkara, M. Challacombe, P.M.W. Gill, B. Johnson, W. Chen, M.W. Wong, C. Gonzalez, J.A. Pople, Gaussian 03, Revision C.02, Gaussian Inc., Wallingford, CT, 2004.
[21] Y. Sasaki, M. Handa, K. Kurashima, T. Tonuma, K. Usamib, J. Electrochem. Soc. 1489 (2001) A999.
[22] C.J. Cramer, G.R. Famini, A.H. Lowrey, Acc. Chem. Res. 26 (1993) 599.
[23] M. Ue, S. Mori, J. Electrochem. Soc. 141 (1994) 3336.
[24] Z.M. Xue, W. Zhou, J. Ding, C.H. Chen, Electrochim. Acta 55 (2010) 5342.
[25] J.B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods, 2nd ed., Gaussian, Pittsburgh, PA, 1996.