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(54) Title: SALTS FOR USE IN ELECTROLYTE COMPOSITIONS OR AS ELECTRODE ADDITIVES

(57) Abstract: The present disclosure relates to compounds for use as electrode additives or as salts in electrolyte compositions, and their methods of preparation. The majority of compounds are anions of imidazoles bearing a sulphonyl or a carbonyl group, or other nitrogen-containing conjugated with various heterocyclic or sulfonyl groups. Also described are some electrochemical cells comprising the compounds as electrode additives or as salts in electrolyte compositions.

SALTS FOR USE IN ELECTROLYTE COMPOSITIONS OR AS ELECTRODE ADDITIVES

RELATED APPLICATION

This application claims priority to United States provisional application No. 62/477,161 filed on March 27th, 2017, the content of which is incorporated herein by reference in its entirety for all purposes.

TECHNICAL FIELD

The technical field generally relates to salts for use in electrolyte compositions or as additive in electrode material, and to methods for the preparation. The technical field also relates to electrolyte compositions and electrode materials containing such salts and to batteries containing them.

BACKGROUND

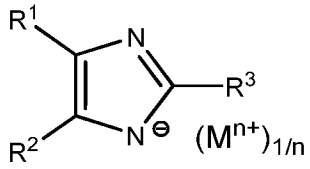
Battery electrolytes, being either liquid, gel or solid, generally consists in one or more lithium salts dissolved in a solvent and/or a solvating polymer. Additives may also further be added to improve the electrolyte's properties, e.g. its stability. Some of these salts may also be included in an electrode material to improve ionic conductivity of the material. Among the salts generally used, $LiPF_6$ (lithium hexafluorophosphate) possesses interesting properties, but degrades in the presence of water to form hydrofluoric acid (HF). This HF formed may result in a dissolution of the cathode material.

Other salts were also developed, including LiFSI and LiTFSI as well as LiTDI. These salts also have their own drawbacks. For example, the $TFSI^-$ anion is very reactive and often leads to the corrosion of the aluminum current collector even at low voltage. Both LiFSI and LiTFSI are not recommended for high voltage applications and are expensive. LiTDI is more stable than the other two but is very hygroscopic and has conductivity and solubility issues.

Therefore, it is highly desirable to develop new salts for use in electrolyte compositions or as additives in electrode materials, for instance, having one or more of the following advantages compared to currently used salts: improved ionic conductivity, lower production costs, improved solubility in electrolyte solvents, and/or the formation of a more conductive SEI.

SUMMARY

According to one aspect, here is described a compound, for instance a salt, for use in electrolyte compositions and/or as additive in electrode materials. In one embodiment, the compound is as defined in Formula I:



Formula I

wherein,

R^1 and R^2 are independently selected from H, F, CN, NO_2, optionally substituted alkyl, preferably CN;

R^3 is selected from $NHSO_2R^4$, $NHSO_2OR^4$, $SO_2NHSO_2R^4$, $SO_2NHSO_2OR^4$ or an optionally substituted heterocycle;

R^4 is selected from fluorine, optionally substituted $C_{1\text{-}6}$alkyl, and optionally substituted C_6aryl;

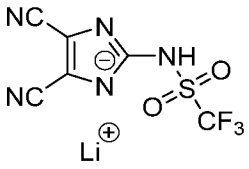
$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

or a tautomer thereof.

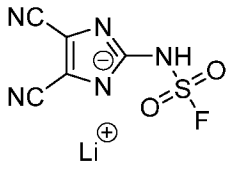
In one embodiment, R^3 is $NHSO_2R^4$. In another embodiment, R^3 is $NHSO_2OR^4$. For instance, R^4 is a $C_{1\text{-}6}$alkyl substituted with at least one of fluorine and alkoxy, or R^4 is a C_6aryl substituted with at least one fluorine atom. In another embodiment,

R^3 is a heterocycle. In another embodiment, at least one of R^1 and R^2 is CN, or both of R^1 and R^2 are CN.

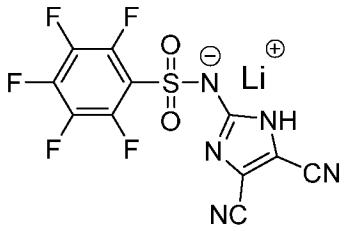
In a further embodiment, the compound of Formula I is compound is selected from:



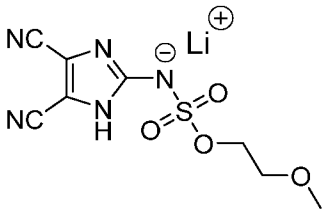
Compound A1



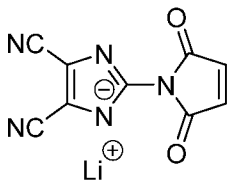
Compound A2



Compound A3



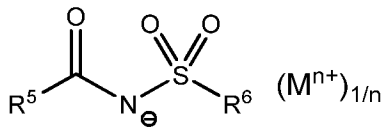
Compound A4



Compound A5

or a tautomer thereof.

According to another embodiment, the compound is as defined in Formula II:



Formula II

wherein,

R^5 is selected from optionally substituted C_{1-6}alkyl and optionally substituted C_6aryl; and

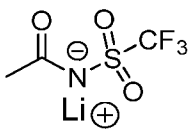
R^6 is selected from optionally substituted C_{1-6}alkyl and optionally substituted C_6aryl;

$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

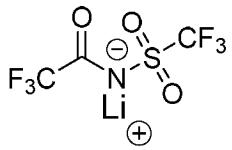
or a tautomer thereof.

In one embodiment, R^5 is an unsubstituted C_{1-6}alkyl group. In another embodiment, R^5 is a fluorinated C_{1-6}alkyl group. In a further embodiment, R^6 is a fluorinated C_{1-6}alkyl group. In yet another embodiment, R^6 is a fluorinated C_6aryl group. In yet another embodiment, at least one of R^5 and R^6 is an optionally substituted C_6aryl group (e.g. a C_6aryl group substituted with one or more fluorine atoms). In other embodiments, the compound is of Formula II, provided that when R^6 is trifluoromethyl, then R^5 is other than methyl or trifluoromethyl.

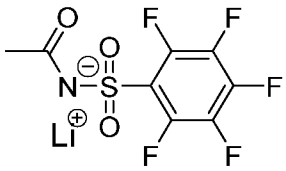
In a further embodiment, the compound of Formula II is compound is selected from:



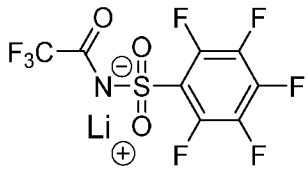
Compound B1



Compound B2



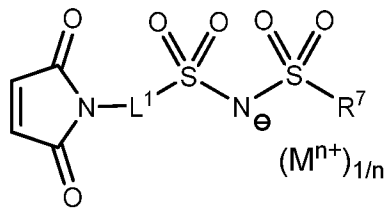
Compound B3



Compound B4

or a tautomer thereof.

According to a further embodiment, the compound is as defined in Formula III:



Formula III

wherein,

R^7 is selected from a fluorine atom and optionally substituted C_{1-6}alkyl; and

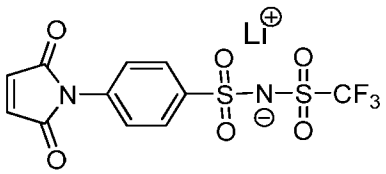
L^1 is a covalent bond or a linker selected from optionally substituted C_{1-6}alkyl and optionally substituted C_6aryl;

$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

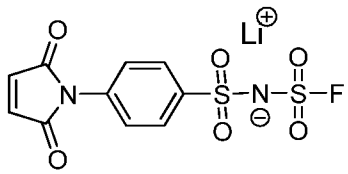
or a tautomer thereof.

In one embodiment, R^7 is a fluorine atom. In another embodiment, R^7 is selected from fluorine substituted C_{1-6}alkyl groups. In a further embodiment, L^1 is a covalent bond or L^1 is a linker selected from optionally substituted C_6aryl groups.

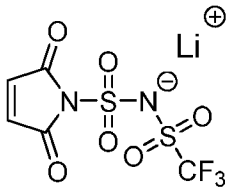
In a further embodiment, the compound of Formula III is compound is selected from:



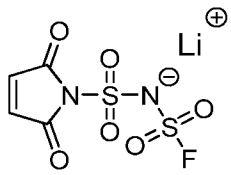
Compound C1



Compound C2



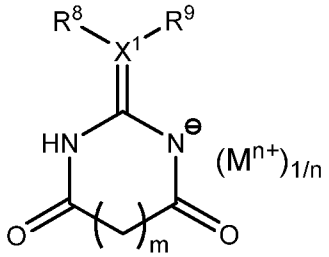
Compound C3



Compound C4

or a tautomer thereof.

According to another embodiment, the compound is as defined in Formula IV:



Formula IV

wherein,

X^1 is a carbon or nitrogen atom;

R^8 and R^9 are each independently F, CN or optionally substituted C_{1-6}alkyl when X^1 is a carbon atom; or

R^8 is absent and R^9 is an optionally substituted SO_2Alkyl or optionally substituted C_{1-6}alkyl when X^1 is a nitrogen atom;

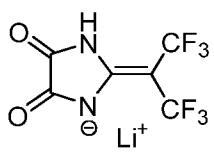
$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

m is an integer selected from 0 or 1;

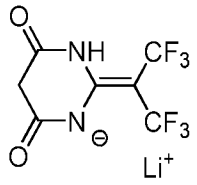
or a tautomer thereof.

In one embodiment, X^1 is a carbon atom. In one embodiment, R^8 and R^9 are different. Alternatively, R^8 and R^9 are the same. In another embodiment, at least one of R^8 and R^9 is CN or optionally substituted C_{1-6}alkyl. In one embodiment, R^8 and R^9 are both CN or optionally substituted C_{1-6}alkyl, or R^8 and R^9 are both CN, or R^8 and R^9 are both fluorine substituted C_{1-6}alkyl. In another embodiment, X^1 is a nitrogen atom. For example, X^1 is a nitrogen atom and R^9 is a fluorine substituted SO_2Alkyl (e.g. SO_2CF_3). In another embodiment, m is 0. In a further embodiment m is 1.

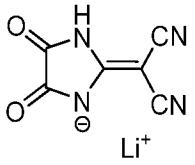
In a further embodiment, the compound of Formula IV is compound is selected from:



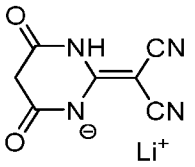
Compound D1



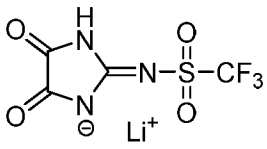
Compound D2



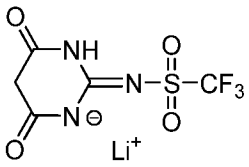
Compound D3



Compound D4



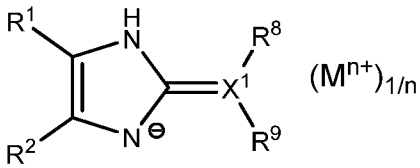
Compound D5



Compound D6

or a tautomer thereof.

According to yet another embodiment, the compound is as defined in Formula V:



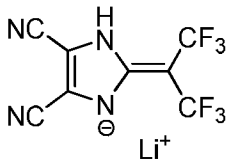
Formula V

wherein, R^1, R^2, R^8, R^9, X^1, M and n are as previously defined, or R^8 and R^9 are absent and X^1 is an oxygen atom;

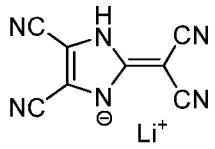
or a tautomer thereof.

In one embodiment, at least one of R^1 and R^2 is CN. For example, both of R^1 and R^2 are CN. In another embodiment, X^1 is a carbon atom. For example, X^1 is a carbon atom and R^8 and R^9 are both CN or optionally substituted $C_{1\text{-}6}$alkyl, or X^1 is a carbon atom and R^8 and R^9 are both CN, or X^1 is a carbon atom and R^8 and R^9 are both fluorine substituted $C_{1\text{-}6}$alkyl. In another embodiment, X^1 is a nitrogen atom. For instance, X^1 is a nitrogen atom and R^9 is a fluorine substituted SO_2Alkyl (e.g. SO_2CF_3).

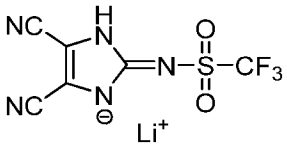
In a further embodiment, the compound of Formula V is compound is selected from:



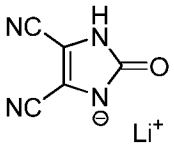
Compound E1



Compound E2



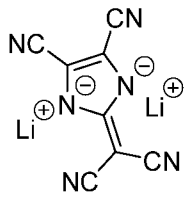
Compound E3



Compound E4

or a tautomer thereof.

In one embodiment, described is a compound according to any one of the foregoing embodiments, wherein M is Li and n is 1. In another embodiment, the compound is as herein defined and is a di-salt (e.g. a dianion forming a salt with two alkali metal anions, where applicable). For example, the compounds of Formulae I, IV and V, the compound may include a further anion on a second nitrogen atom. For instance, Compounds E1 to E4 may form a disalt, such as, for compound E2:



Further contemplated are the free forms of any of the salts referred to herein.

According to another aspect, the present technology relates to an electrode material comprising, as an additive, a compound as herein defined, and at least one electrochemically active material.

According to another aspect, the present technology relates to an electrolyte composition comprising a compound as herein described. For instance, the electrolyte composition further comprises a compatible solvent. In another example, the electrolyte composition further comprises a compatible solvating polymer.

In a further aspect, also contemplated is an electrochemical cell comprising an electrolyte, an electrode and a counter-electrode, wherein at least one of the electrode or counter-electrode comprises an electrode material comprising, as an additive, a compound as herein defined, and at least one electrochemically active material. Alternatively, contemplated is an electrochemical cell which comprises an electrolyte composition comprising a compound as herein defined, an electrode and a counter-electrode. In one embodiment, the electrochemical cell comprises a compound as herein defined in an electrolyte composition and in at least one electrode material. In one embodiment, electrochemical cell is included in a battery, an electrochromic device, or a capacitor. For instance, the battery is a lithium or lithium-ion battery. In other examples, the battery is a sodium or potassium battery.

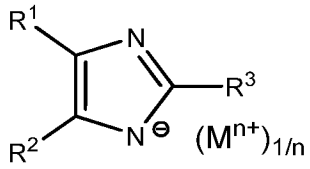
According to another aspect, described in the use of the electrochemical cell as herein defined in electrical or hybrid vehicles, or in ubiquitous IT devices.

Other features and advantages of the present technology will be better understood upon reading of the description herein below.

DETAILED DESCRIPTION

Here are described compounds (e.g. salts) intended for use as electrode material additives or as a component of an electrolyte composition. Compounds described are of one of Formulae I to V as herein defined. Exemplary compounds are also described and should not be interpreted as limiting the scope of the broader formulae.

Accordingly, the compound may be as defined in Formula I:



Formula I

wherein,

R^1 and R^2 are independently selected from H, F, CN, NO_2, optionally substituted alkyl, preferably CN;

R^3 is selected from $NHSO_2R^4$, $NHSO_2OR^4$, $SO_2NHSO_2R^4$, $SO_2NHSO_2OR^4$ or an optionally substituted heterocycle;

R^4 is selected from fluorine, optionally substituted C_{1-6}alkyl, and optionally substituted C_6aryl;

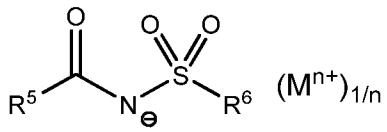
$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

or a tautomer thereof.

For example, R^3 is $NHSO_2R^4$, or R^3 is $NHSO_2OR^4$. For instance, R^3 is $NHSO_2R^4$ or $NHSO_2OR^4$ and R^4 is a C_{1-6}alkyl substituted with at least one of fluorine and alkoxy, or R^4 is a C_6aryl substituted with at least one fluorine atom. In another example, R^3 is a C_{5-6}heterocycle (e.g. a non-aromatic C_{5-6}heterocycle linked through a nitrogen atom, such as a maleimide). In another embodiment, at least one of R^1 and R^2 is CN, or both of R^1 and R^2 are CN.

Examples of compounds of Formula I include, without limitation, Compounds A1 to A5 a defined above, or a tautomer thereof.

The compound may also be defined as in Formula II:



Formula II

wherein,

R^5 is selected from optionally substituted C_{1-6}alkyl and optionally substituted C_6aryl; and

R^6 is selected from optionally substituted C_{1-6}alkyl and optionally substituted C_6aryl;

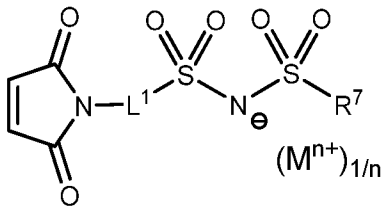
$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

or a tautomer thereof.

For example, R^5 is an unsubstituted C_{1-6}alkyl group (such as methyl, ethyl, propyl, isopropyl and the like), or R^5 is a fluorinated C_{1-6}alkyl group (e.g. trifluoromethyl, and the like). In another example, R^6 is a fluorinated C_{1-6}alkyl group (e.g. trifluoromethyl, and the like) or R^6 is a fluorinated C_6aryl group (e.g. pentafluorophenyl, and the like). Other examples include compounds of Formula II wherein at least one of R^5 and R^6 is an optionally substituted C_6aryl group. In other examples, the compound is of Formula II, provided that when R^6 is trifluoromethyl, then R^5 is other than methyl or trifluoromethyl.

Examples of compounds of Formula II include, without limitation, Compounds B1 to B4, as herein defined, or a tautomer thereof. For instance, the compound is Compounds B3 or B4, as herein defined, or a tautomer thereof.

The compound may also be as defined in Formula III:



Formula III

wherein,

R^7 is selected from a fluorine atom and optionally substituted C_{1-6}alkyl; and

L^1 is a covalent bond or a linker selected from optionally substituted C_{1-6}alkyl and optionally substituted C_6aryl;

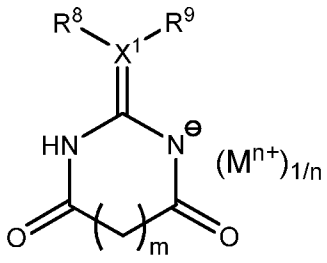
$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

or a tautomer thereof.

For example, R^7 is a fluorine atom or R^7 is selected from fluorine substituted C_{1-6}alkyl groups. According to some examples, L^1 is a covalent bond. According to other examples, L^1 is a linker selected from optionally substituted C_6aryl groups.

Examples of compounds of Formula III include, without limitation, Compounds C1 to C4, as herein defined, or a tautomer thereof.

The compound may further be defined as in Formula IV:



Formula IV

wherein,

X^1 is a carbon or nitrogen atom;

R^8 and R^9 are each independently F, CN or optionally substituted C_{1-6}alkyl when X^1 is a carbon atom; or

R^8 is absent and R^9 is an optionally substituted SO_2Alkyl or optionally substituted C_{1-6}alkyl when X^1 is a nitrogen atom;

$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

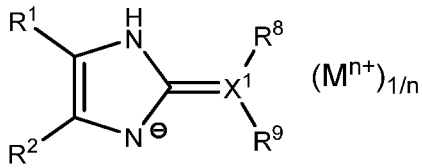
m is an integer selected from 0 or 1;

or a tautomer thereof.

In some examples, X^1 is a carbon atom. When X^1 is a carbon atom, R^8 and R^9 may be the same or different. For instance, X^1 is a carbon atom and at least one of R^8 and R^9 is CN or optionally substituted $C_{1\text{-}6}$alkyl. For instance, X^1 is a carbon atom and R^8 and R^9 are both CN or optionally substituted $C_{1\text{-}6}$alkyl, or R^8 and R^9 are both CN, or R^8 and R^9 are both fluorine substituted $C_{1\text{-}6}$alkyl. According to other examples, X^1 is a nitrogen atom. For example, X^1 is a nitrogen atom, R^8 is absent and R^9 is a fluorine substituted SO_2Alkyl (e.g. SO_2CF_3). In one example, m is 0. In a further example, m is 1.

Examples of compounds of Formula IV include, without limitation, Compounds D1 to D6, as herein defined, or a tautomer thereof.

The compound may also further be defined as in Formula V:



Formula V

wherein, R^1, R^2, R^8, R^9, X^1, M and n are as previously defined, or R^8 and R^9 are absent and X^1 is an oxygen atom;

or a tautomer thereof.

For example, at least one of R^1 and R^2 is CN, or both of R^1 and R^2 are CN. In some examples, X^1 is a carbon atom. For instance, X^1 is a carbon atom and R^8 and R^9 are both CN or optionally substituted $C_{1\text{-}6}$alkyl, or X^1 is a carbon atom and R^8 and

R^9 are both CN, or X^1 is a carbon atom and R^8 and R^9 are both fluorine substituted C_{1-6}alkyl. In other examples, X^1 is a nitrogen atom. For instance, X^1 is a nitrogen atom and R^9 is a fluorine substituted SO_2Alkyl (e.g. SO_2CF_3).

Examples of compounds of Formula V include, without limitation, Compounds E1 to E4, as herein defined, or a tautomer thereof.

According to one example, the compound is as defined in any one of Formulae I to V, wherein M is Li and n is 1. In another embodiment, the compound is as herein defined and is a di-salt (e.g. a dianion forming a salt with two alkali metal anions, where applicable). For example, the compounds of Formulae I, IV and V, the compound may include a further anion on a second nitrogen atom. Further contemplated are the free forms of any of the salts referred to herein.

As used herein, the term “alkyl” refers to saturated hydrocarbons having from one to sixteen carbon atoms, including linear or branched alkyl groups. Examples of alkyl groups include, without limitation, methyl, ethyl, propyl, butyl, pentyl, hexyl, heptyl, octyl, nonyl, decyl, isopropyl, *tert*-butyl, *sec*-butyl, isobutyl, and the like. When the alkyl group is located between two functional groups, then the term alkyl also encompasses alkylene groups such as methylene, ethylene, propylene, and the like. The term “C_1-$C_n$alkyl” refers to an alkyl group having from 1 to the indicated “n” number of carbon atoms.

The term “alkoxy” as used herein means an alkyl group having an oxygen atom attached thereto. Representative alkoxy groups include groups having 1 to about 6 carbon atoms, *e.g.,* methoxy, ethoxy, propoxy, *tert*-butoxy and the like. Examples of alkoxy groups include methoxy, ethoxy, isopropyloxy, propoxy, butoxy, pentoxy, fluoromethoxy, difluoromethoxy, trifluoromethoxy, chloromethoxy, dichloromethoxy, trichloromethoxy groups and the like. The term alkoxy includes both unsubstituted or substituted alkoxy groups, etc., as well as halogenated alkyloxy groups.

The term “aryl” refers to aromatic groups having 4n+2 π(pi) electrons, wherein n is an integer from 1 to 3, in a conjugated monocyclic or polycyclic system (fused or not) and having six to fourteen ring atoms. A polycyclic ring system includes at least one aromatic ring. Aryl may be directly attached, or connected via a C_1-C_3alkyl group (also referred to as arylalkyl or aralkyl). Examples of aryl groups include, without limitation, phenyl, benzyl, phenethyl, 1-phenylethyl, tolyl, naphthyl, biphenyl, terphenyl, indenyl, benzocyclooctenyl, benzocycloheptenyl, azulenyl, acenaphthylenyl, fluorenyl, phenanthrenyl, anthracenyl, and the like. The term aryl includes both unsubstituted aryl groups and substituted aryl groups. The term “C_6-$C_n$aryl” refers to an aryl group having from 6 to the indicated “n” number of carbons in the ring structure.

The terms “heterocycle” or “heterocyclic” include heterocycloalkyl and heteroaryl groups. Examples of heterocycles include, without limitation, acridinyl, azocinyl, benzimidazolyl, benzofuranyl, benzothiofuranyl, benzothiophenyl, benzoxazolyl, benzthiazolyl, benztriazolyl, benztetrazolyl, benzisoxazolyl, benzisothiazolyl, benzimidazolinyl, carbazolyl, 4αH-carbazolyl, carbolinyl, chromanyl, chromenyl, cinnolinyl, decahydroquinolinyl, 2H,6H-1,5,2-dithiazinyl, dihydrofuro[2,3-b]tetrahydrofuran, furanyl, furazanyl, imidazolidinyl, imidazolinyl, imidazolyl, 1H-indazolyl, indolenyl, indolinyl, indolizinyl, indolyl, 3H-indolyl, isobenzofuranyl, isochromanyl, isoindazolyl, isoindolinyl, isoindolyl, isoquinolinyl, isothiazolyl, isoxazolyl, methylenedioxyphenyl, morpholinyl, naphthyridinyl, octahydroisoquinolinyl, oxadiazolyl, 1,2,3-oxadiazolyl, 1,2,4-oxadiazolyl, 1,2,5-oxadiazolyl, 1,3,4-oxadiazolyl, oxazolidinyl, oxazolyl, oxazolidinyl, pyrimidinyl, phenanthridinyl, phenanthrolinyl, phenazinyl, phenothiazinyl, phenoxathiinyl, phenoxazinyl, phthalazinyl, piperazinyl, piperidinyl, piperidonyl, 4-piperidonyl, piperonyl, pteridinyl, purinyl, pyranyl, pyrazinyl, pyrazolidinyl, pyrazolinyl, pyrazolyl, pyridazinyl, pyridooxazole, pyridoimidazole, pyridothiazole, pyridinyl, pyridyl, pyrimidinyl, pyrrolidinyl, pyrrolinyl, 2H-pyrrolyl, pyrrolyl, quinazolinyl, quinolinyl, 4H-quinolizinyl, quinoxalinyl, quinuclidinyl, tetrahydrofuranyl, tetrahydroisoquinolinyl, tetrahydroquinolinyl, tetrazolyl,

6H-1,2,5-thiadiazinyl, 1,2,3-thiadiazolyl, 1,2,4-thiadiazolyl, 1,2,5-thiadiazolyl, 1,3,4-thiadiazolyl, thianthrenyl, thiazolyl, thienyl, thienothiazolyl, thienooxazolyl, thienoimidazolyl, thiophenyl, triazinyl, 1,2,3-triazolyl, 1,2,4-triazolyl, 1,2,5-triazolyl, 1,3,4-triazolyl, xanthenyl, and the like. The term heterocycle includes both unsubstituted heterocyclic groups and substituted heterocyclic groups.

The term "substituted", when in association with any of the foregoing groups refers to a group substituted at one or more position with substituents such as cyano, halogen, nitro, trifluoromethyl, lower alkyl, cycloalkyl, heterocycloalkyl, aryl, heteroaryl, lower alkoxy, aryloxy, benzyloxy, benzyl, sulfonyl, sulfonate, sulfonamide, phosphonato, phosphinato, oxo, and the like. Any of the above substituents can be further substituted if permissible, e.g. if the group contains an alkyl group, an alkoxy group, an aryl group, or other.

Also described is an electrode material comprising, as an additive, a compound as herein defined, and at least one electrochemically active material. The electrochemically active material may be a material for use in a negative electrode. Alternatively, the electrochemically active material may be a material for use in a positive electrode. Examples of electrochemically active materials include, without limitation, titanates and lithium titanates (e.g. TiO_2, Li_2TiO_3, $Li_4Ti_5O_{12}$, $H_2Ti_5O_{11}$, $H_2Ti_4O_9$, or a combination thereof), lithium and metal phosphates (e.g. $LiM'PO_4$ where M' is Fe, Ni, Mn, Co, or a combination thereof), vanadium oxides (e.g. LiV_3O_8, V_2O_5, LiV_2O_5, and the like), and other lithium and metal oxides such as $LiMn_2O_4$, $LiM''O_2$ (M'' being Mn, Co, Ni, or a combination thereof), $Li(NiM''')O_2$ (M''' being Mn, Co, Al, Fe, Cr, Ti, Zr, and the like, or a combination thereof), or a combination thereof. For instance, the active material is selected from Lithium iron phosphate (LFP), lithium manganese iron phosphate (LMFP), lithium titanate (LTO), graphite, and lithium nickel manganese cobalt oxide (NMC). The particles may be freshly formed or of commercial source, in the form of microparticles or nanoparticles and may further include a carbon coating.

The electrode material may also optionally include additional components like conductive materials, inorganic particles, glass or ceramic particles, and the like. Examples of conductive materials include carbon black, Ketjen™ black, acetylene black, graphite, graphene, carbon fibers, nanofibers (e.g. VGCF) or nanotubes, or a combination thereof. The electrode material may also further comprise a binder. Examples of binders include water soluble binders such as SBR (styrene butadiene rubber), NBR (butadiene acrylonitrile rubber), HNBR (hydrogenated NBR), CHR (epichlorohydrin rubber), ACM (acrylate rubber), and the like, and cellulose-based binders (e.g. carboxyalkylcellulose, hydroxyalkylcellulose, and combinations), or any combination of two or more of these. For instance, the carboxyalkylcellulose may be carboxymethylcellulose (CMC) or carboxyethylcellulose. Hydroxypropylcellulose is an example of hydroxyalkylcellulose. Other examples of binders include fluorine-containing polymeric binders such as PVDF and PTFE, and ion-conductive polymer binders such as block copolymers composed of at least one lithium-ion solvating segment and at least one cross-linkable segment.

According to another aspect, the present technology relates to an electrolyte composition comprising a compound as herein described. The electrolyte may be a liquid, gel or solid polymer electrolyte and, in the case of a lithium or lithium-ion electrochemical cell, is conductive to lithium ions. For instance, the electrolyte composition further comprises a compatible solvent. In another example, the electrolyte composition further comprises a compatible solvating polymer.

For example, electrolytes are prepared by dissolution of one or more of the present compounds in an appropriate electrolyte solvent or solvating polymer for polymer electrolyte preparation. For use in lithium and lithium ion batteries, the compounds as lithium salts can be dissolved at an appropriate concentration, for example between 0.05 and 3 mol/litre. For other types of batteries, other salts of the present compounds should be dissolved, for example, sodium salts for sodium batteries, magnesium salts for magnesium batteries, and the like.

Non-limiting examples of electrolyte solvents include organic solvents such as ethers, carbonate esters, cyclic carbonate esters, aliphatic carboxylic acid esters, aromatic carboxylic acid esters, phosphate esters, sulfite esters, nitriles, amides, alcohols, sulfoxides, sulfolane, nitromethane, 1,3-dimethyl-2-imidazolidinone, 1,3-diméthyl-3,4,5,6-tetrahydro-2(1,H)-pyrimidinone, 3-methyl-2-oxazolidinone, or a mixture thereof. In particular examples, the solvent may also be an aqueous solvent, i.e. water or a mixture comprising water.

Examples of solvents include dimethyl carbonate, diethyl carbonate, ethyl methyl carbonate, propylene carbonate, ethylene carbonate, γ-butyrolactone, glyme, diglyme, triglyme, tetraglyme, sulfolane, tetraethylsulfamide, acetonitrile, pyruvonitrile, propionitrile, methoxypropionitrile, dimethylaminopropionitrile, butyronitrile, isobutyronitrile, valeronitrile, pivalonitrile, isovaléronitrile, glutaronitrile, méthoxyglutaronitrile, 2-methylglutaronitrile, 3-methylglutaronitrile, adiponitrile, malononitrile, and combinations thereof. Various additives may also be included in the electrolyte composition to improve its properties.

Non-limiting examples of polymers for use in electrolytes (e.g. gel or solid) include poly(ethylene oxide) and its copolymers and block-copolymers, poly(propylene oxide) and its copolymers and block-copolymers, poly(dimethylsiloxane) and its copolymers and block-copolymers, poly(alkylene carbonate) and their copolymers and block-copolymers, poly(alkylenesulfone) and its copolymers and block-copolymers, poly(alkylenesulfamides) and its copolymers and block-copolymers, polyurethanes and their copolymers and block-copolymers, poly(vinylalcohol) and its copolymers and block-copolymers and combinations thereof. Additionally, branched or cross-linked solvating polymers may also be included. Various additives may also be included in the polymer electrolyte composition to improve its properties.

Electrochemical cells as herein described comprise an electrolyte, an electrode and a counter-electrode, wherein at least one of the electrode or counter-electrode comprises an electrode material comprising, as an additive, a compound as herein

defined, and at least one electrochemically active material as defined above. Alternatively, contemplated is an electrochemical cell which comprises an electrolyte composition comprising a compound as herein defined, an electrode and a counter-electrode. In one embodiment, the electrochemical cell comprises a compound as herein defined in an electrolyte composition and in at least one electrode material. In one embodiment, the electrochemical cell is included in a battery, an electrochromic device, or a capacitor. For instance, the battery is a lithium or lithium-ion battery. In other examples, the battery is a sodium or potassium battery.

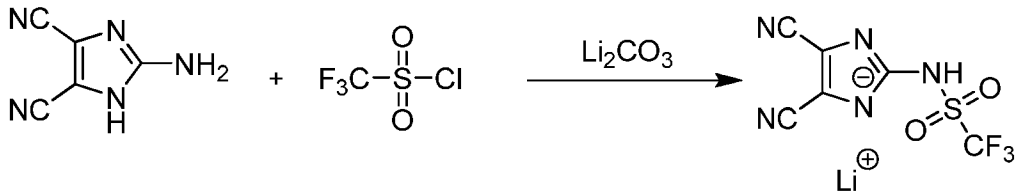
According to another aspect, described in the use of the electrochemical cell as herein defined in electrical or hybrid vehicles, or in ubiquitous IT devices.

EXAMPLES

The following non-limiting examples are illustrative embodiments and should not be construed as further limiting the scope of the present application.

Example 1: Preparation of Compounds of Formula I

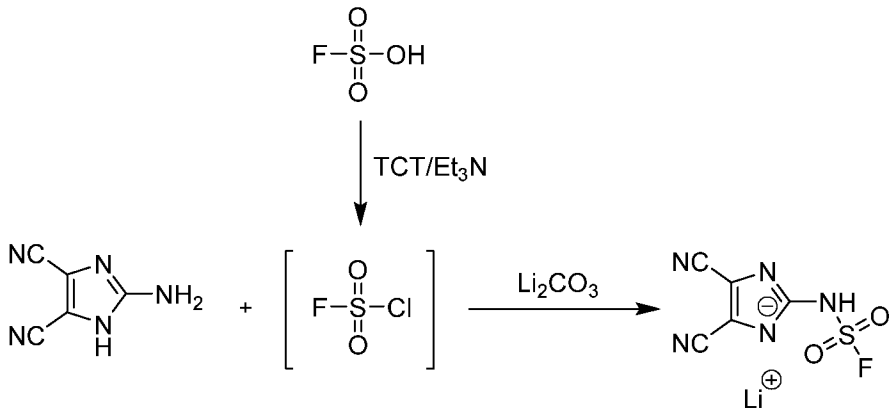
a) Compound A1



2-Amino-1H-imidazole-4,5-dicarbonitrile (1.1 eq), trifluorosulfonylchloride (1 eq), lithium carbonate (2 eq) and N'N-dimethylaminopyridine (DMAP) (0.25 eq) were introduced in a Schlenk flask. The solids were degassed by vacuum-N_2 cycles. Dry acetone (1M) was added and the suspension was vigorously stirred and heated under reflux overnight. The reaction mixture was cooled down to room temperature. Distilled water was added, and the solution was extracted using dichloromethane. The combined organic layers were washed with water and acidic water, dried using $MgSO_4$ and filtered. The solution was filtered on Celite® to

eliminate inorganic residues. The organic solution was concentrated under reduced pressure until dryness. The solid residue was purified by silica gel chromatography using hexanes/ethyl acetate (1/1) as eluent. A crystalline yellow solid was isolated after evaporation. This yellow solid was then dissolved in water and monohydrated lithium hydroxide was added until a slight excess of base was detected using a pH paper. The solution was concentrated until dryness by reduced pressure distillation. The solid was suspended in diethyl carbonate (DEC) and stirred overnight at room temperature. The solution was passed through Celite® and the clear solution was concentrated under reduced pressure and dried in a vacuum oven for 24 hours.

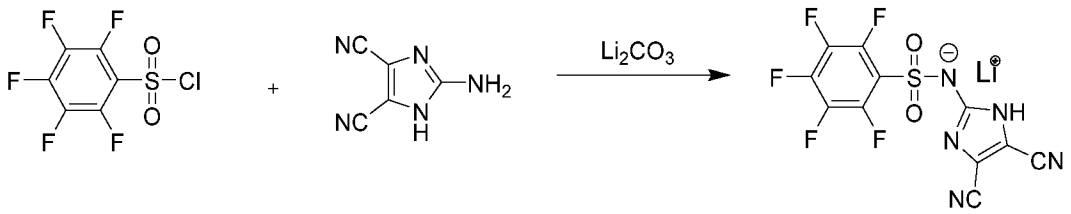
b) Compound A2



2,4,6-Trichloro-[1,3,5]-triazine (1 eq.) was added to a room temperature solution of sulfonic acid (1 eq.) in dry acetone, followed by trimethylamine (1 eq.) dropwise. The solution was stirred vigorously and heated at 90°C overnight. The reaction mixture was cooled to room temperature and, under nitrogen, 2-amino-1H-imidazole-4,5-dicarbonitrile (1.2 eq.), DMAP (0.25 eq.) and lithium carbonate (2 eq.) were added. The mixture was stirred vigorously and heated at 90°C for 2 days. The reaction mixture was cooled down to room temperature. Distilled water was added, and the solution was extracted using dichloromethane. The combined organic layers were washed with water and acidic water, dried using $MgSO_4$ and filtered. The solution was filtered on Celite® to eliminate inorganic residues. The organic solution was concentrated under reduced pressure until dryness. The solid

residue was purified by silica gel chromatography using hexanes/ethyl acetate (1/1) as eluent. A crystalline yellow solid was isolated. The yellow solid was then dissolved in water and monohydrated lithium hydroxide was added until a slight excess of base was detected using a pH paper. The solution was concentrated until dryness by reduced pressure distillation. The solid was suspended in diethyl carbonate (DEC) and stirred overnight at room temperature. The solution was passed through Celite® and the clear solution was concentrated under reduced pressure and dried in a vacuum oven for 24 hours.

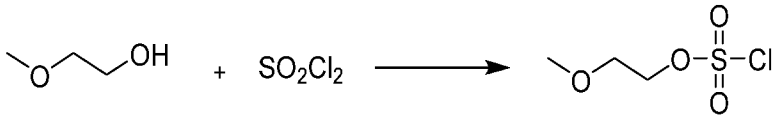
c) Compound A3



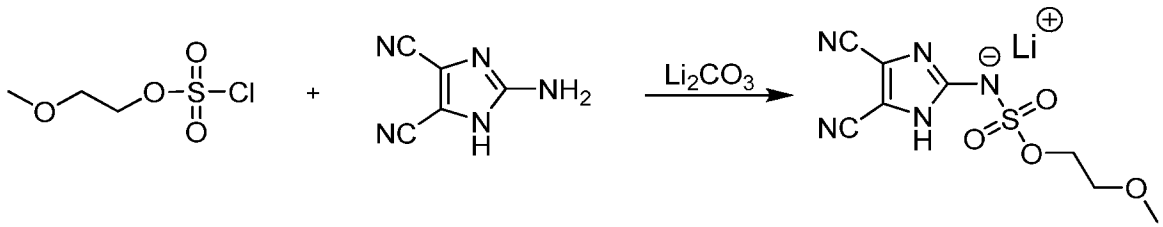
2-Amino-1H-imidazole-4,5-dicarbonitrile (1.1 eq), pentafluorosulfonylchloride (1 eq), lithium carbonate (2 eq) and N'N-dimethylaminopyridine (DMAP) (0.25 eq) were introduced in a Schlenk flask. The solids were degassed by vacuum-N_2 cycles. Dry acetone (1M) was added and the suspension was vigorously stirred and heated under reflux. The reaction mixture was cooled down to room temperature. Distilled water was added, and the solution was extracted using dichloromethane. The combined organic layers were washed with water and acidic water, dried using $MgSO_4$ and filtered. The solution was filtered on Celite® to eliminate inorganic residues. The organic solution was concentrated under reduced pressure until dryness. The solid residue was purified by silica gel chromatography using hexanes/ethyl acetate (1/1) as eluent. A crystalline yellow solid was isolated. The yellow solid was then dissolved in water and monohydrated lithium hydroxide was added until a slight excess of base was detected using a pH paper. The solution was concentrated until dryness by reduced pressure distillation. The solid was suspended in diethyl carbonate (DEC) and stirred overnight at room temperature. The solution was passed through Celite® and the

clear solution was concentrated under reduced pressure and dried in a vacuum oven for 24 hours.

d) Compound A4



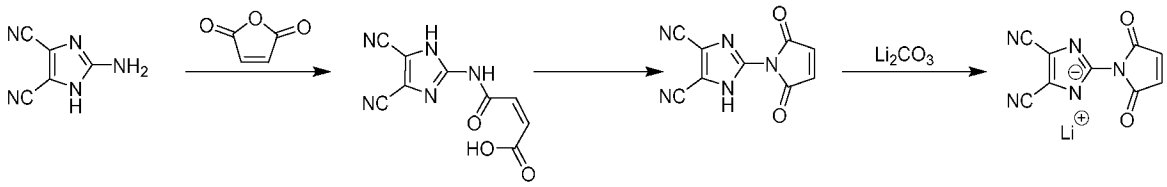
Step 1: A solution of 2-methoxyethan-1-ol in THF was added dropwise to a solution of sulfuryl chloride (1.2 eq) in THF at -75°C. The reaction mixture was warmed up to room temperature. The solution was concentrated until dryness under reduced pressure. The colorless oil obtained was used without purification.



Step 2: 2-amino-1H-imidazole-4,5-dicarbonitrile (1.1 eq), 2-methoxyethan-1-sulfonylchloride (1 eq), lithium carbonate (2 eq) and N'N-dimethylaminopyridine (DMAP) (0.25 eq) were introduced in a Schlenk flask. The solids were degassed by vacuum-N_2 cycles. Dry acetone (1M) was added and the suspension was stirred vigorously and heated under reflux overnight. The reaction mixture was cooled to room temperature. Distilled water was added and the resulting solution was extracted using dichloromethane. The organic layers were combined, washed with water and acidic water, dried on $MgSO_4$ and filtered. The organic solution obtained was concentrated under reduced pressure until dryness. The resulting brown oil was purified by silica gel chromatography. A yellow oil was isolated. The resulting compound was converted to its lithium salt by dissolution in water and addition of lithium hydroxide. The solution was concentrated until dryness by reduced pressure distillation. The solid was suspended in diethyl carbonate (DEC) and stirred overnight at room temperature. The solution was passed through Celite®

and the clear solution was concentrated under reduced pressure and dried in a vacuum oven for 24 hours.

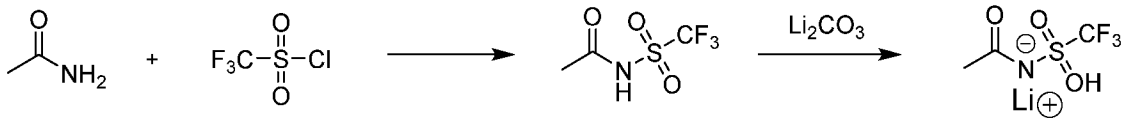
e) Compound A5



2-amino-1H-imidazole-4,5-dicarbonitrile and maleic anhydride were dissolved in 1,4-dioxane. The solution was heated at 150°C during 10 hours by microwaves activation. The mixture was precipitated in cold diethyl ether and filtrated. The yellowish filtrate was evaporated, and a pale yellow highly hydroscopic solid was isolated. The solid was then dissolved in water and monohydrated lithium hydroxide was added until a slight excess of base was detected using a pH paper. The solution was concentrated until dryness by reduced pressure distillation. The solid was suspended in diethyl carbonate (DEC) and stirred overnight at room temperature. The solution was passed through Celite® and the clear solution was concentrated under reduced pressure and dried in a vacuum oven for 24 hours.

Example 2: Preparation of Compounds of Formula II

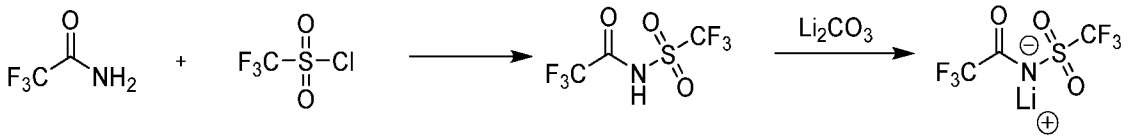
a) Compound B1



Acetamide (1.1 eq), trifluorosulfonylchloride (1 eq), lithium carbonate (2 eq) and N'N-dimethylaminopyridine (DMAP) (0.25 eq) were introduced in a Schlenk flask. The solids were degassed by vacuum-N_2 cycles. Dry acetone (1M) was added and the suspension was stirred vigorously and heated under reflux overnight. The reaction mixture was cooled down to room temperature. Distilled water was added, and the solution was extracted using dichloromethane. The combined organic phases were washed with water, dried on $MgSO_4$ and filtered. The organic solution

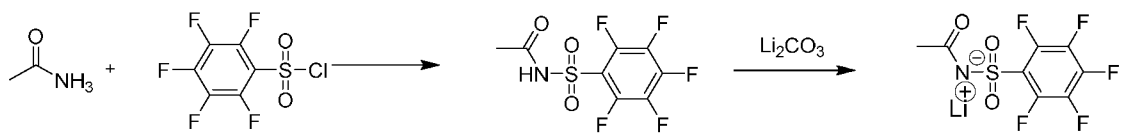
was concentrated to dryness under reduced pressure. The crude oil was then dissolved in water and monohydrated lithium hydroxide was added until a slight excess of base was detected using a pH paper. The solution was concentrated until dryness by reduced pressure distillation. The solid was suspended in diethyl carbonate (DEC) and stirred overnight at room temperature. The solution was passed through Celite® and the clear solution was concentrated under reduced pressure and dried in a vacuum oven for 24 hours.

b) Compound B2



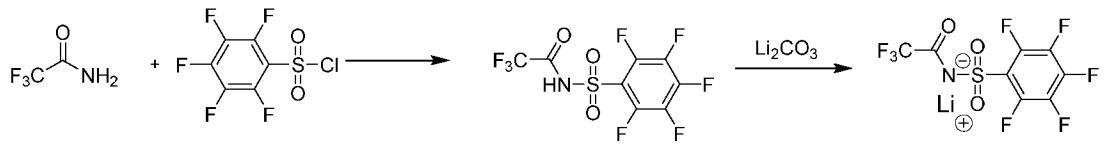
Trifluorocetamide (1.1 eq), trifluorosulfonylchloride (1 eq), lithium carbonate (2 eq) and N'N-dimethylaminopyridine (DMAP) (0.25 eq) were introduced in a Schlenk flask. The solids were degassed by vacuum-N_2 cycles. Dry acetone (1M) was added and the suspension was stirred vigorously and heated under reflux overnight. The reaction mixture was cooled to room temperature. Distilled water was added, and the solution was extracted using dichloromethane. The organic layers were combined, washed with water, dried on $MgSO_4$ and filtered. The organic solution was concentrated to dryness under reduced pressure. The crude oil was then dissolved in water and monohydrated lithium hydroxide was added until a slight excess of base was detected using a pH paper. The solution was concentrated until dryness by reduced pressure distillation. The solid was suspended in diethyl carbonate (DEC) and stirred overnight at room temperature. The solution was passed through Celite® and the clear solution was concentrated under reduce pressure and dried in vacuum oven for 24 hours.

c) Compound B3



Acetamide (1.1 eq), pentafluorobenzenesulfonyl chloride (1 eq), lithium carbonate (2 eq) and N'N-dimethylaminopyridine (DMAP) (0.25 eq) were introduced in a Schlenk flask. The solids were degassed by vacuum-N_2 cycles. Dry acetone (1M) was added and the suspension was stirred vigorously and heated under reflux overnight. The reaction mixture was cooled to room temperature, distilled water was added, and the solution was extracted using dichloromethane. The organic layers were combined, washed with water, dried on $MgSO_4$ and filtered. The crude solid was then dissolved in water and monohydrated lithium hydroxide was added until a slight excess of base was detected using a pH paper. The solution was concentrated until dryness by reduced pressure distillation. The solid was suspended in diethyl carbonate (DEC) and stirred overnight at room temperature. The solution was passed through Celite® and the clear solution was concentrated under reduced pressure and dried in a vacuum oven for 24 hours.

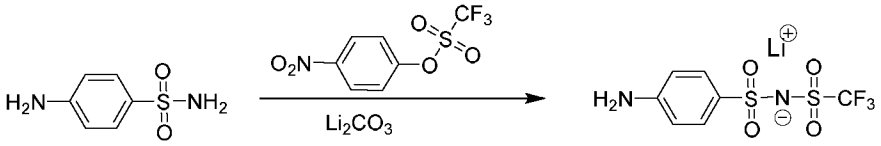
d) Compound B4



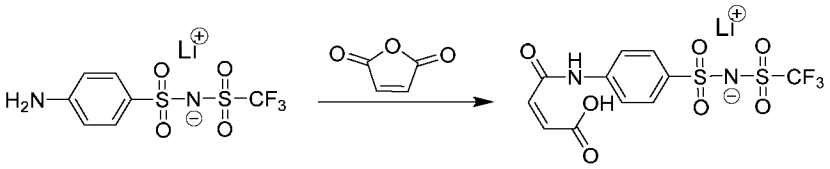
Trifulorocetamide (1.1 eq), pentafluorobenzenesulfonyl chloride (1 eq), lithium carbonate (2 eq) and N'N-dimethylaminopyridine (DMAP) (0.25 eq) were introduced in a Schlenk flask. The solids were degassed by vacuum-N_2 cycles. Dry acetone (1M) was added and the suspension was stirred vigorously and heated under reflux overnight. The reaction mixture was cooled to room temperature, distilled water was added, and the solution was extracted using dichloromethane. The organic layers were combined, washed with water, dried on $MgSO_4$ and filtered. The crude solid was then dissolved in water and monohydrated lithium hydroxide was added until a slight excess of base was detected using a pH paper. The solution was concentrated until dryness by reduced pressure distillation. The solid was suspended in diethyl carbonate (DEC) and stirred overnight at room temperature. The solution was passed on Celite® and the clear solution was concentrated under reduce pressure and dried in vacuum oven for 24 hours.

Example 3: Preparation of Compounds of Formula III

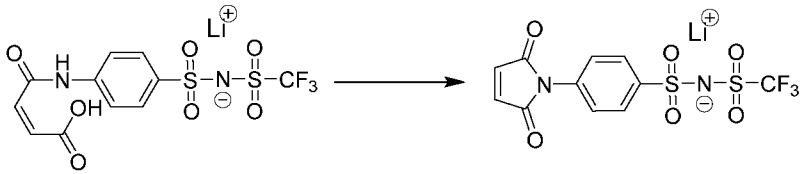
Compound C1



Step 1: Sulfanilamide, lithium carbonate (1 eq.) and 4-nitrophenyl trifluoromethanesulfonate were mixed and ground using a mortar and pestle. The molten mixture was stirred at 180°C for one hour under nitrogen. Deionized water was added to the hot mixture under vigorous stirring. The insoluble suspended solid was removed by filtration. Water was removed under reduced pressure. The solid was washed with cold THF, ethyl acetate and a white solid was filtered. The yellow filtrate was evaporated under reduce pressure and the yellow solid was dried overnight at 40°C under vacuum.



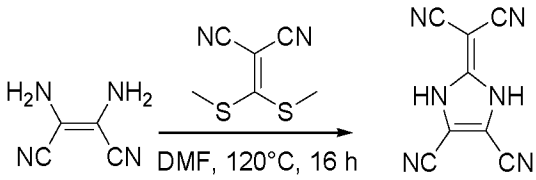
Step 2: A THF solution of the solid from step 1 was added to a solution of maleic anhydride in 1,4-dioxane and the resulting mixture was stirred at room temperature for 12 hours. The corresponding carboxylic acid was isolated as a white solid by filtration and was dried under vacuum at 60°C for 4 hours.



Step 3: A acetic anhydride solution of the carboxylic acid from step 2 and sodium acetate was heated at 70°C for 3 hours. Then, the solution was poured into an excess of diethyl ether to complete the precipitation. The resulting precipitate was isolated by filtration and dried under vacuum at 60°C overnight.

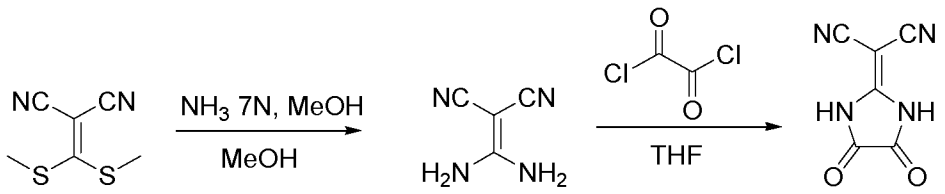
Example 4: Preparation of Compounds of Formulae IV and V

a) Compound E2 (free form)



A solution of diaminomaleonitrile (1.0 g, 4.625 mmol) and anhydrous dimethylformamide (10 mL) is added to an inert reactor. The compound 2-[bis(methylthio)methylene]malononitrile (DM3) (0.787 g, 4.625 mmol) is added and the mixture stirred for 16 hours at 120°C. Solvents and volatile compounds are removed under vacuum. The resulting product is purified by silica-gel chromatography using a mixture of ethyl acetate and hexanes as eluent.

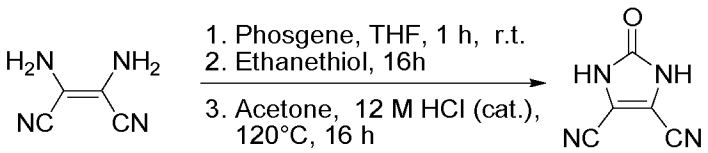
b) Compound D3 (free form)



A solution of compound DM3 (0.500 g, 2.94 mmol) in methanol (50 mL) is inserted into an inert reactor (pressure bomb). Ammonia (0.500 g, 29.4 mmol) is added and the reaction mixture is stirred for 16 hours at 70°C. Solvent and volatile compounds are removed under vacuum. The compound obtained (DM3-NH_2) is used without further purification.

A solution of compound DM3-NH_2 (0.500 g, 4.63 mmol) in THF (50 mL) is introduced in an inert reactor. Oxalyl chloride (0.587 g, 4.63 mmol) is added and the reaction mixture is stirred for 16 hours at room temperature. The solvent and volatile compounds are removed under vacuum. The product is purified by recrystallization in alcohols.

c) Compound E4 (free form)



A solution of diaminomaleonitrile (8.0 g, 74.0 mmol) in anhydrous tetrahydrofuran (250 mL) is introduced in an inert reactor and the solution is degassed. Phosgene (7.32 g, 74.0 mmol) is added and the mixture is stirred for 1 hour. Ethanethiol (14.9 g, 148.0 mmol) is then added and the mixture is stirred for another 16 h. The solvent and volatile compounds are removed under vacuum. Acetone (100 mL) and 5 drops of 12 M HCl are added and the mixture is heated for 16 h at 120°C until a complete discoloration from orange to grey-white is observed. The product is a grey-white powder.

Example 5: Conductivity of selected salts

Conductivity measurements were carried out with a biologic conductivity meter (model MCS-10) using a platinum cell (type HTCC: parallel plates platinized platinum on glass holder). The salts were dried in a vacuum oven at 70°C for one night prior to use, and PC/EMC/DMC (4/3/3) or distilled water were used as solvent. Solutions of LiCl (in water) or $LiPF_6$ (in PC/EMC/DMC) were used as references.

Table 1. Conductivity results

Compound	Concentration (mol/L)	Conductivity (mS/cm)	Reference	Concentration (mol/L)	Conductivity (mS/cm)
A1	0.1M	0.64	$LiPF_6$	0.1M	2.96
A2	0.3M	0.63	$LiPF_6$	0.3M	6.78
A5	0.1M	0.04	$LiPF_6$	0.1M	2.96
A5	0.1M	21.66	LiCl	0.1M	9.75
E2*	0.1M	9.71	LiCl	0.1M	9.75

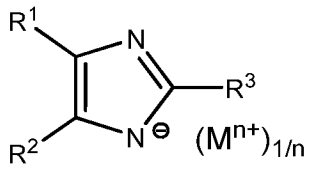
* In its di-lithium salt form.

Numerous modifications could be made to any of the embodiments described above without departing from the scope of the present invention. Any references,

patents or scientific literature documents referred to in this application are incorporated herein by reference in their entirety for all purposes.

CLAIMS

1. A compound as defined in Formula I:



Formula I

wherein,

R^1 and R^2 are independently selected from H, F, CN, NO_2, optionally substituted alkyl, preferably CN;

R^3 is selected from $NHSO_2R^4$, $NHSO_2OR^4$, $SO_2NHSO_2R^4$, $SO_2NHSO_2OR^4$ or an optionally substituted heterocycle;

R^4 is selected from fluorine, optionally substituted C_{1-6}alkyl, and optionally substituted C_6aryl;

$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

or a tautomer thereof.

2. The compound of claim 1, wherein R^3 is $NHSO_2R^4$.

3. The compound of claim 1, wherein R^3 is $NHSO_2OR^4$.

4. The compound of claim 2 or 3, wherein R^4 is a C_{1-6}alkyl substituted with at least one of fluorine and alkoxy.

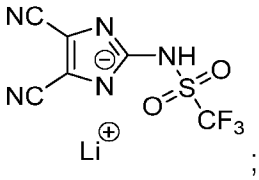
5. The compound of claim 2 or 3, wherein R^4 is a C_6aryl substituted with at least one fluorine atom.

6. The compound of claim 1, wherein R^3 is a heterocycle.

7. The compound of any one of claims 1 to 6, wherein at least one of R^1 and R^2 is CN.

8. The compound of claim 7, wherein both of R^1 and R^2 are CN.

9. The compound of claim 1, wherein said compound is selected from: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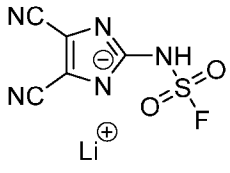
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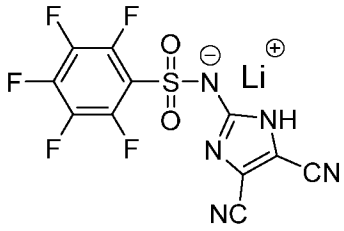
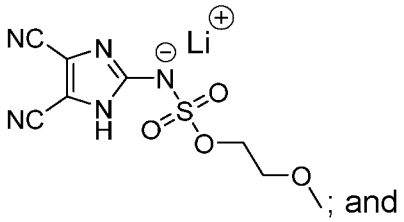
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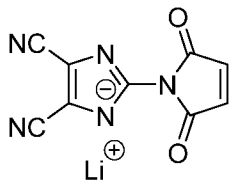
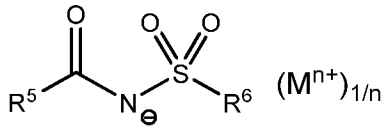

;

or a tautomer thereof.

10. A compound as defined in Formula II:



Formula II

wherein,

R^5 is selected from optionally substituted $C_{1\text{-}6}$alkyl and optionally substituted C_6aryl; and

R^6 is selected from optionally substituted $C_{1\text{-}6}$alkyl and optionally substituted C_6aryl;

$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

or a tautomer thereof.

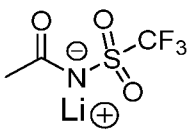
11. The compound of claim 10, wherein R^5 is an unsubstituted C_{1-6}alkyl group.

12. The compound of claim 10, wherein R^5 is a fluorinated C_{1-6}alkyl group.

13. The compound of any one of claims 10 to 12, wherein R^6 is a fluorinated C_{1-6}alkyl group.

14. The compound of any one of claims 10 to 12, wherein R^6 is a fluorinated C_6aryl group.

15. The compound of claim 10, wherein said compound is selected from: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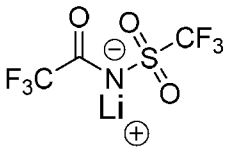
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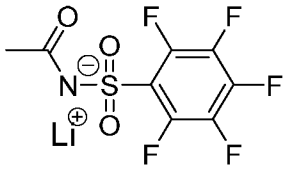
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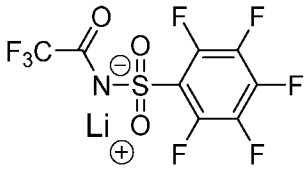
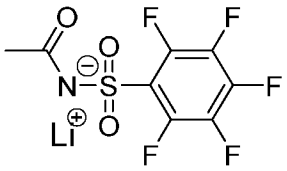
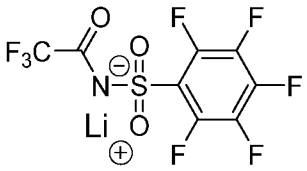
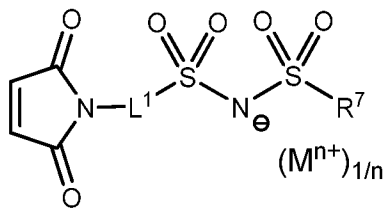

;

or a tautomer thereof.

16. The compound of claim 15, wherein said compound is selected from:


or

.

17. A compound as defined in Formula III:



Formula III

wherein,

R^7 is selected from a fluorine atom and optionally substituted C_{1-6}alkyl; and

L^1 is a covalent bond or a linker selected from optionally substituted C_{1-6}alkyl and optionally substituted C_6aryl;

$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

or a tautomer thereof.

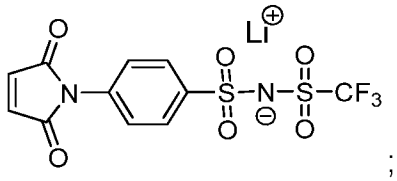
18. The compound of claim 17, wherein R^7 is a fluorine atom.

19. The compound of claim 17, wherein R^7 is selected from fluorine substituted C_{1-6}alkyl groups.

20. The compound of any one of claims 17 to 19, wherein L^1 is a covalent bond.

21. The compound of any one of claims 17 to 19, wherein L^1 is a linker selected from optionally substituted C_6aryl groups.

22. The compound of claim 17, wherein said compound is selected from: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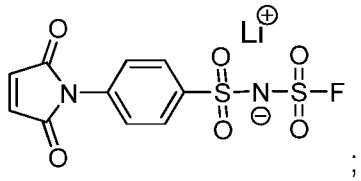
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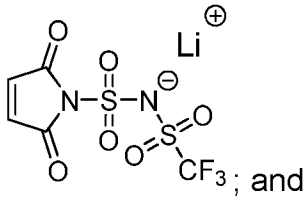
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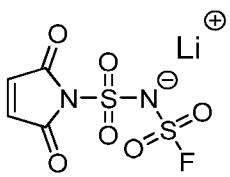
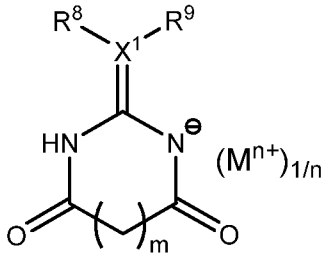

;

or a tautomer thereof.

23. A compound as defined in Formula IV:



Formula IV

wherein,

X^1 is a carbon or nitrogen atom;

R^8 and R^9 are each independently F, CN or optionally substituted C_{1-6}alkyl when X^1 is a carbon atom; or

R^8 is absent and R^9 is an optionally substituted SO_2Alkyl or optionally substituted C_{1-6}alkyl when X^1 is a nitrogen atom;

$(M^{n+})_{1/n}$ is a metal cation, wherein M is a metal and n is 1 or 2, for instance M is an alkali metal, alkaline earth metal, for instance, M is Li, Na, or K, or M is Li and n is 1;

m is an integer selected from 0 or 1;

or a tautomer thereof.

24. The compound of claim 23, wherein X^1 is a carbon atom.

25. The compound of claim 24, wherein at least one of R^8 and R^9 is CN or optionally substituted C_{1-6}alkyl

26. The compound of claim 24 or 25, wherein R^8 and R^9 are both CN or optionally substituted C_{1-6}alkyl.

27. The compound of claim 24 or 25, wherein R^8 and R^9 are both CN.

28. The compound of claim 24 or 25, wherein R^8 and R^9 are both fluorine substituted C_{1-6}alkyl.

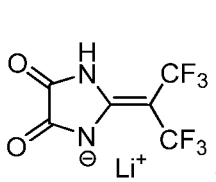
29. The compound of claim 23, wherein X^1 is a nitrogen atom.

30. The compound of claim 29, wherein R^9 is a fluorine substituted SO_2Alkyl (e.g. SO_2CF_3).

31. The compound of any one of claims 23 to 30, wherein m is 0.

32. The compound of any one of claims 23 to 30, wherein m is 1.

33. The compound of claim 23, wherein said compound is selected from: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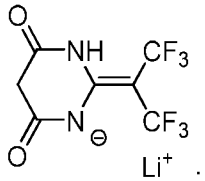
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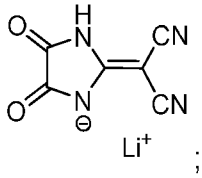
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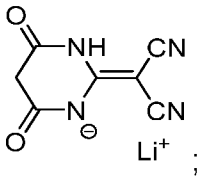
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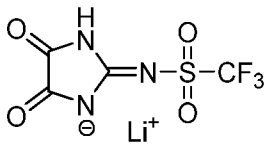
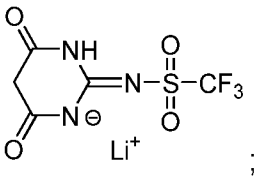

; and

;

or a tautomer thereof.

34. A compound as defined in Formula V:

Formula V

wherein, R^1, R^2, R^8, R^9, X^1, M and n are as previously defined, or R^8 and R^9 are absent and X^1 is an oxygen atom;

or a tautomer thereof.

35. The compound of claim 34, wherein at least one of R^1 and R^2 is CN.

36. The compound of claim 35, wherein both of R^1 and R^2 are CN.

37. The compound of any one of claims 34 to 36, wherein X^1 is a carbon atom.

38. The compound of claim 37, wherein at least one of R^8 and R^9 is CN or optionally substituted C_{1-6}alkyl.

39. The compound of claim 37, wherein R^8 and R^9 are both CN or optionally substituted C_{1-6}alkyl.

40. The compound of claim 37, wherein R^8 and R^9 are both CN.

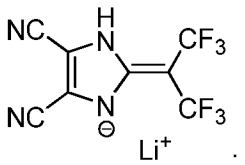
41. The compound of claim 37, wherein R^8 and R^9 are both fluorine substituted C_{1-6}alkyl.

42. The compound of any one of claims 34 to 36, wherein X^1 is a nitrogen atom.

43. The compound of claim 42, wherein R^9 is a fluorine substituted SO_2Alkyl (e.g. SO_2CF_3).

44. The compound of any one of claims 1 to 43, wherein M is Li and n is 1.

45. The compound of claim 34, wherein said compound is selected from:



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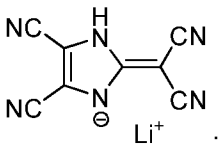

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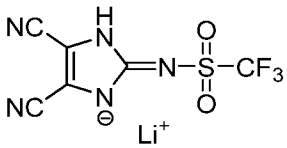
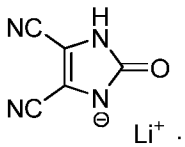


; and


;

or a tautomer thereof.

46. Electrode material comprising a compound as defined in any one of claims 1 to 45 as an additive and at least one electrochemically active material.

47. An electrolyte composition comprising a compound as defined in any one of claims 1 to 45.

48. The electrolyte composition of claim 47, further comprising a compatible solvent.

49. The electrolyte composition of claim 48, wherein the compatible solvent is an organic solvent.

50. The electrolyte composition of claim 48, wherein the compatible solvent is an aqueous solvent.

51. The electrolyte composition of claim 47, further comprising a compatible solvating polymer.

52. An electrochemical cell comprising an electrolyte, an electrode and a counter-electrode, wherein at least one of the electrode or counter-electrode comprises an electrode material as defined in claim 46.

53. An electrochemical cell comprising an electrolyte as defined in any one of claims 47 to 51, an electrode and a counter-electrode.

54. The electrochemical cell of claim 52 or 53, wherein said electrochemical cell is a battery, an electrochromic device, or a capacitor.

55. The electrochemical cell of claim 54, wherein said battery is a lithium or lithium-ion battery.

56. Use of the electrochemical cell of any one of claims 52 to 55 in electrical or hybrid vehicles, or in ubiquitous IT devices.

INTERNATIONAL SEARCH REPORT

International application No.
PCT/CA2018/050370

A. CLASSIFICATION OF SUBJECT MATTER
IPC: ***C07D 233/90*** (2006.01) , ***C07C 311/51*** (2006.01) , ***C07D 207/448*** (2006.01) , ***C07D 233/96*** (2006.01) , ***C07D 239/54*** (2006.01) , ***C07D 403/04*** (2006.01) ***H01M 10/0567*** (2010.01) , ***H01M 4/13*** (2010.01) , ***H01M 4/62*** (2006.01)

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
C07D 233/90 (2006.01) , ***C07D 207/448*** (2006.01)

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic database(s) consulted during the international search (name of database(s) and, where practicable, search terms used)
STN, Canadian Patent Database
Search terms: imidazol*; electrod*; anion

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	CA 2,248,246 C (C. MICHOT et al.) 9 July 1998 (09-07-1998) Examples 4, 5, 14, 32; claims	1-9 and 46-56
X	CA 2,194,127 A1 (C. MICHOT et al.) 30 June 1998 (30-06-1998) Figures 3.61-3.65, 3.74; page 108; claims 3-5	1-9 and 46-56
X	CA 2,925,554 A1 (G. SCHMIDT et al.) 9 April 2015 (09-04-2015) Formula (I); claims 1 and 16	1-9 and 46-56

☐ Further documents are listed in the continuation of Box C.

☑ See patent family annex.

*	Special categories of cited documents:
"A"	document defining the general state of the art which is not considered to be of particular relevance
"E"	earlier application or patent but published on or after the international filing date
"L"	document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O"	document referring to an oral disclosure, use, exhibition or other means
"P"	document published prior to the international filing date but later than the priority date claimed
"T"	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X"	document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y"	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"&"	document member of the same patent family

Date of the actual completion of the international search 17 May 2018 (17-05-2018)	Date of mailing of the international search report 18 June 2018 (18-06-2018)
Name and mailing address of the ISA/CA Canadian Intellectual Property Office Place du Portage I, C114 - 1st Floor, Box PCT 50 Victoria Street Gatineau, Quebec K1A 0C9 Facsimile No.: 819-953-2476	Authorized officer Denis Bélanger (819) 639-8703

INTERNATIONAL SEARCH REPORT

International application No.
PCT/CA2018/050370

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of the first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claim Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☐ Claim Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. ☐ Claim Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box No. III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:

Invention 1 Imidazoles of formula (I) : claims 1-9 and 46-56 (partially)
Invention 2 Compounds of formula (II) : claims 10-16 and 46-56 (partially)
Invention 3 Compounds of formula (III) : claims 17-22 and 46-56 (partially)
Invention 4 Compounds of formula (IV) : claims 23-33 and 46-56 (partially)
Invention 5 Compounds of formula (V) : claims 34-45 and 46-56 (partially)

Continuation on Extra sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. ☐ As all searchable claims could be searched without effort justifying additional fees, this Authority did not invite payment of additional fees.

3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claim Nos.:

4. ☑ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claim Nos.: 1-9 and 46-56

Remark on Protest

☐ The additional search fees were accompanied by the applicant's protest and, where applicable, the payment of a protest fee.

☐ The additional search fees were accompanied by the applicant's protest but the applicable protest fee was not paid within the time limit specified in the invitation.

☐ No protest accompanied the payment of additional search fees.

Continuation of Box III :

In Group 1 of inventions, the core structure is an imidazole ring system adjacent to a sulfonyl group;
in Group 2 of inventions, the core structure is a sulphonamide adjacent to a carbonyl group;
in Group 3 of inventions, the core structure is a sulphonamide linked to a second sulfonyl group;
in Group 4 of inventions, the core structure is a double lactam without a sulfonyl group;
and in Group 5 of inventions, the core structure is an imidazole ring system without a sulfonyl group.

Consequently, the five groups of invention are not so linked to form a unitary general inventive concept.

Patent Document Cited in Search Report	Publication Date	Patent Family Member(s)	Publication Date
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		CA2248246C	09 February 2010 (09-02-2010)
		AU6971181A	28 October 1982 (28-10-1982)
		CA2194127A1	30 June 1998 (30-06-1998)
		CA2199231A1	05 September 1998 (05-09-1998)
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		EP0035850A1	16 September 1981 (16-09-1981)
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