Supplementary Information (SI) for Sustainable Energy & Fuels.

Intercalation and De-intercalation Mechanism in Lithium Metal Fluorosulfate-based Half and Full-Cell Configurations: A DFT Study

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Results and discussion

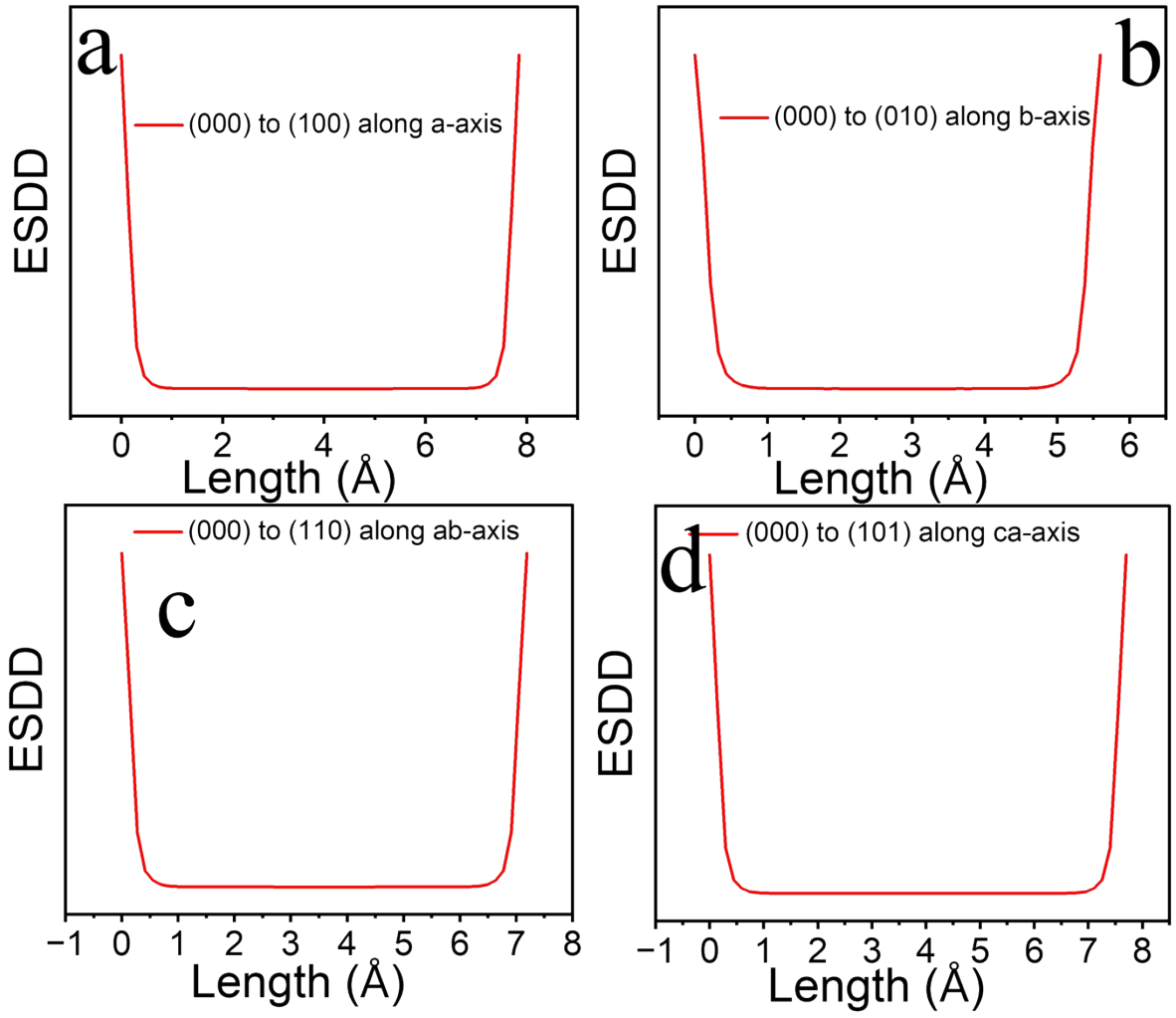

Figure S1. Line profile of Li-ion diffusion: a) along a-axis, b) along b-axis, c) along ab-axis, d) along ab-axis.

Table T1. Diffusion distance and activation energies of LFCS along different directions

LFCS	Diffusion distance (Å)	Activation energy (E_a, eV)
Along a-axis	7.53	1.6
Along b-axis	5.30	1.01
Along c-axis	3.6	0.2
Along ab-axis	6.92	1.1
Along ac-axis	7.4	1.3

Thermal properties

LFCS

Internal energy (E) = -195.565 Ha, Pressure = 9.315 GPa, T = 300 K, V = 193.039 $Å^3$, K_B = 1.380649 $x10^{-23}$ J/K

Entropy = (-479.346275x 4.35974 $x10^{-18}$)/(1.380649 $x10^{-18}$ x 300)

Entropy = - 5.046 J/K

H=E + PV

= -195.565 x 27.211396 eV + ((9.315 x 193.039 $Å^3$)/160.21766208 $Å^3$)

= -5321.5967 + 11.2232213 = -5310.37348 eV

G= H-TS = -5310.37348 eV - (300 K x - 5.046 J/K) = 1513.8 J

= 1513.8 J

FCS

Internal energy (E) = -140.634 Ha, Pressure = 5.950 GPa, T = 300 K, V = 185.048 $Å^3$, K_B = 1.380649 $x10^{-23}$ J/K

Entropy = (-665.188 x 4.35974 $x10^{-18}$)/(1.380649 $x10^{-18}$ x 300)

Entropy = - 7.002 J/K

H=E + PV

= -140.634 x 27.211396 eV + ((5.950 x 185.048 $Å^3$)/160.21766208 $Å^3$)

= -3826.84747 + 6.8721 = -3819.97537 eV

= -3819.975 eV

G= H-TS = -3819.975 eV + (300 K x 7.002 J/K) = 2100.6 J

= 2100.6 J

$\Delta G = G_f - G_i$ = 2100.6 J - 1513.8 J = 586.8 J

= 586.8 J (+ve)

LFMS

Internal energy (E) = -242.947 Ha, Pressure = -10.757 GPa, T = 300 K, V = 196.217 $Å^3$, K_B = 1.380649×10^{-23} J/K

Entropy = $(-455.1147 \times 4.35974 \times 10^{-18})/(1.380649 \times 10^{-18} \times 300)$

Entropy = -4.79045667 J/K

H=E + PV

= -242.947 x 27.211396 eV + ((10.757 x 196.217 $Å^3$)/160.21766208 $Å^3$)

= -6610.92702 + 13.1739924 = -6597.733 eV

G= H-TS = -6597.733 eV - (300 K x - 4.79045667 J/K)

= -1437.137 J

FMS

Internal energy (E) = -212.839 Ha, Pressure = -11.120 GPa, T = 300 K, V = 182.154 $Å^3$, K_B = 1.380649×10^{-23} J/K

Entropy = $(-559.6493 \times 4.35974 \times 10^{-18})/(1.380649 \times 10^{-18} \times 300)$

Entropy = -5.89076 J/K

H=E + PV

= -212.839 x 27.211396 eV + ((11.120 x 182.154 $Å^3$)/160.21766208 $Å^3$)

= -5791.64631 + 12.6425 = -5779.00381 eV

G= H-TS = -5779.00381 eV - (300 K x - 5.89076 J/K)

= -1767.228 J

LFNS,

Internal energy (E) = -309.003 Ha, Pressure = - 9.6467 GPa, T = 300 K, V = 192.809 $Å^3$, K_B = 1.380649 $x10^{-23}$ J/K

Entropy = (-393.278 x 4.35974 $x10^{-18}$)/(1.380649 $x10^{-18}$ x 300)

Entropy = -4.13957 J/K

H=E + PV

= -309.003 x 27.211396 eV + ((9.6467 x 192.809 $Å^3$)/160.21766208 $Å^3$)

= -8408.403 + 11.609 = -8396.794 eV

G= H-TS = - 8396.794 eV - (300 K x - 4.13957 J/K) = 1241.871 J

= 1241.871 J

FNS

Internal energy (E) = -298.979 Ha, Pressure = - 8.7607 GPa, T = 300 K, V = 191.568 $Å^3$, K_B = 1.380649 $x10^{-23}$ J/K

Entropy = (-494.576 x 4.35974 $x10^{-18}$)/(1.380649 $x10^{-18}$ x 300)

Entropy = -5.206 J/K

H=E + PV

= -298.979 x 27.211396 eV + ((8.7607 x 191.568 $Å^3$)/160.21766208 $Å^3$)

= -8135.6359 + 10.4749361 = -8125.1609 eV

G= H-TS = -8125.1609 eV - (300 K x - 5.206 J/K)

= 1561.8 J

Electrochemical properties calculations

The average voltage of LFCS in regard to Li metal is represented by way of

$V = -[E(LFCS) - E(FCS) - E(Li)]/F$ -----Eqn.1

where E is the average energy of a completely stress-free ground-level structure, and F is the Faraday constant.

Single-electron oxidation voltage (V_{ox}) related to the Li^+/Li reference electrode was measured as follows:

V_{ox} (vs. Li+/Li) = [E(LFCS) − E(FCS) − E(Li)]/F+ $E_{SCE\ /SHE}$ − $E_{(Li+/Li)/SHE}$ -----Eqn.2

where F is Faraday's constant. $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/Li)/SHE}$ (-3.04 V) are the potentials of an electron in a vacuum and of a metallic lithium electrode

Reduction potential is given as

V_{rx} (vs. Li^+/Li) = [E(LFCS) − E(FCS) − E(Li)]/F − $E_{\circ(Li+/Li)/SCE}$ ----- Eqn.3

where M′ = Mn, Fe, Ni, F is Faraday's constant. $E_{(Li+/Li)/SCE}$ (-3.04 V) are the potentials of metallic lithium with respect to saturated calomel electrode

The average volumetric energy density is expressed as

Ω = − [E(LFCS) − E(FCS) − E(Li)]/V_{av} -----Eqn.4

where Vav is the average volume of the fully relaxed ground state structure.

The gravimetric energy density is proposed as

γ = − [E(LFCS) − E(FCS) − E(Li)]/m_{av} -----Eqn.5

where m_{av} is the average mass of a completely stress-free ground-level structure

The theoretical specific capacity of an anode material can be expressed by Faraday's law:

$Q_{theoretical}$ = (nF) / (3600*Mw) mA h g^{-1} -----Eqn.6

Where n is the number of charge carriers, F is the Faraday constant, F=26.801×10^3 mA h mol^{-1} and Mw is the molecular weight of the active material [1, 4].

LFCS

The average voltage of LFCS with respect to Li metal is represented as

V = − [E(LFCS) − E(FCS) − E(Li)]/F -----Eqn. (1)

where E is the average energy of fully relaxed ground state structure, F is the Faraday constant.

V=-[((-425.6134)-(-215.648)-(-204.976)) eV]/(96.5 kJ/mol)

V= 4.9894 V ~ 4.99 V

Single-electron oxidation voltage (V_{ox}) related to the Li^+/Li reference electrode was measured as follows:

V_{ox} (vs. Li+/Li) = [E(LFCS) − E(FCS)- E(Li)]/F+ $E_{SCE\ /SHE}$ + $E_{(Li+/Li)/SHE}$ Eqn. S19

where F is Faraday's constant. $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/Li)/SHE}$ (−3.04 V) are the potentials of an electron in a vacuum and of a metallic lithium electrode

V_{ox}(vs.Li+/Li)=[(-425.6134)-(-215.648) -(-204.976)]/(96.5kJ/mol)+0.24-3.04 V

V_{ox}(vs.Li+/Li) = 4.989 V +0.24-3.04 V = 2.189 V ~ 2.2 V

Reduction potential is given as

V_{rx} (vs. Li^+/Li) = -[E(LFCS) − E(FCS) - E(Li)]/F + $E_{\circ(Li+/Li)/SCE}$ Eqn. S20

Where F is Faraday's constant. $E_{(Li+/Li)/SCE}$ (-3.04 V) are the potentials of metallic lithium with respect to saturated calomel electrode

V_{ox}(vs.Li+/Li)=-[(-425.6134)-(-215.648) -(-204.976)]/(96.5kJ/mol) - 3.04 V

V_{ox}(vs.Li+/Li) = 4.989 V - 3.04 V = -1.949 V ~ -1.95 V

Average volumetric energy density is given as

$\Omega = -$ [E(LFCS) − E(FCS) − E(Li)]/V_{av}

where Vav is the average volume of the fully relaxed ground state structure.

$\Omega = -$ [((-425.6134) - (-215.648) - (-204.70560196)) eV]/(193.039 $\times 10^{-24}$ cm^3)

Ω = [4.989 x1.602$\times 10^{-19}$ j]/(193.039 $\times 10^{-24}$ cm^3) [1eV=1.602$\times 10^{-19}$ j],

[one joul (J) = 2.77778e-7 kW h]

Ω = [4.989 x 1.602$\times 10^{-19}$ x 2.77778e-7 kW h]/(193.039 $\times 10^{-24}$ cm^3)

Average volumetric energy density (Ω) = 1.15 W h/cm^3

Average volumetric power density = 1.15 W/cm^3

Specific energy is expressed as

$\gamma = -$ [E(LFCS) − E(FCS) − E(Li)]/m_{av} ----------(3)

where m_{av} is the average mass of a fully relaxed ground state structure

γ =−[(-425.6134) - (-215.648) - (-204.70560196)) eV]/(34.39799 g/mol)

[4.989 x96.485kj/mole]/(34.39799 g/mol)

[4.75468x96.485x2.77778 e-4 kW h]/(34.39799 g)

= 3.8872 Wh/g 1eV= 96.485kj/mole, kJ = 2.77778 e-4 kW h

Gravimetric energy density = 3.89 kWh/kg

Gravimetric power density = 3.89 kW/kg

Theoretical capacity

The theoretical capacity of a cathode material can be calculated by Faraday's law:

$Q_{theoretical} = (nF) / (3600*Mw)$ mA h g^{-1} Eqn. S21

Where n is the number of charge carriers, F is the Faraday constant F=26.801×10^3 mA h $mol^{-1}$and Mw is the molecular weight of the active material.

$Q_{theoretical} = (1x26.801\times10^3)/(0.36*351.8379)$ mA h g^{-1}

= 211.595232 mA h g^{-1}

FCS

Theoretical capacity

The theoretical capacity of a cathode material can be calculated by Faraday's law:

$Q_{theoretical} = (nF) / (3600*Mw)$ mA h g^{-1} Eqn. S21

Where n is the number of charge carriers, F is the Faraday constant F=26.801×10^3 mA h $mol^{-1}$and Mw is the molecular weight of the active material.

$Q_{theoretical} = (1x26.801\times10^3)/(0.36*337.955)$ mA h g^{-1} = 220.3 mA h g^{-1}

LFMS

The average voltage of LTO with respect to Li metal is represented as

V = − [E(LFMS) − E(FMS) − E(Li)]/F -----Eqn. (1)

where E is the average energy of fully relaxed ground state structure, F is the Faraday constant.

V=-[((-442.993)-(-232.946)-(-204.976)) eV]/(96.5 kJ/mol)

V= 5.071 V ~ 5.071 V

Single-electron oxidation voltage (V_{ox}) related to the Li^+/Li reference electrode was measured as follows:

V_{ox} (vs. Li+/Li) = [E(LFMS) − E(MCS)- E(Li)]/F+ $E_{SCE\ /SHE}$ + $E_{(Li+/Li)/SHE}$ Eqn. S19

where F is Faraday's constant. $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/Li)/SHE}$ (−3.04 V) are the potentials of an electron in a vacuum and of a metallic lithium electrode

V_{ox}(vs.Li+/Li)=[(-442.993)-(-232.946) -(-204.976)]/(96.5kJ/mol)+0.24-3.04 V

V_{ox}(vs.Li+/Li) = -5.071 V +0.24-3.04 V = 2.271 V

Reduction potential is given as

V_{rx} (vs. Li^+/Li) = -[E(LFMS) − E(FMS) - E(Li)]/F + $E_{\circ(Li+/Li)/SCE}$ Eqn. S20

Where F is Faraday's constant. $E_{(Li+/Li)/SCE}$ (-3.04 V) are the potentials of metallic lithium with respect to saturated calomel electrode

V_{ox}(vs.Li+/Li)=-[(-442.993)-(-232.946) -(-204.976)]/(96.5kJ/mol) - 3.04 V

V_{ox}(vs.Li+/Li) = 5.071 V - 3.04 V = 2.03 V

Average volumetric energy density is given as

Ω = − [E(LFMS) − E(FMS) − E(Li)]/V_{av}

where Vav is the average volume of the fully relaxed ground state structure.

Ω = − [((-442.993) - (-232.946) - (-204.70560196)) eV]/(196.217 ×10^{-24} cm^3)

Ω = [5.071 x1.602×10^{-19} j]/(193.039 ×10^{-24} cm^3) [1eV=1.602×10^{-19} j],

[one joul (J) = 2.77778e-7 kW h]

Ω = [5.071 x 1.602×10^{-19} x 2.77778e-7 kW h]/(196.217 ×10^{-24} cm^3)

Average volumetric energy density (Ω) = 1.15 W h/cm^3

Average volumetric power density = 1.15 W/cm^3

Specific energy is expressed as

γ = − [E(LFMS) − E(FMS) − E(Li)]/m_{av} ----------(3)

where m_{av} is the average mass of a fully relaxed ground state structure

γ =−[(-425.6134) - (-215.648) - (-204.70560196)) eV]/(34.39799 g/mol)

[5.2598x96.485kj/mole]/(35.0533 g/mol)

[4.75468x96.485x2.77778 e-4 kW h]/(34.39799 g)

= 3.705 Wh/g 1eV= 96.485kj/mole, kJ = 2.77778 e-4 kW h

Gravimetric energy density = 3.705 kWh/kg

Gravimetric power density = 3.705 kW/kg

Theoretical capacity

The theoretical capacity of a cathode material can be calculated by Faraday's law:

$Q_{theoretical}$ = (nF) / (3600*Mw) mA h g^{-1} Eqn. S21

Where n is the number of charge carriers, F is the Faraday constant F=26.801×10^3 mA h $mol^{-1}$and Mw is the molecular weight of the active material.

$Q_{theoretical}$ = (1x26.801×10^3)/(0.36*322.749) mA h g^{-1}

= 230.7 mA h g^{-1}

FMS

Theoretical capacity

The theoretical capacity of a cathode material can be calculated by Faraday's law:

$Q_{theoretical}$ = (nF) / (3600*Mw) mA h g^{-1} Eqn. S21

Where n is the number of charge carriers, F is the Faraday constant F=26.801×10^3 mA h $mol^{-1}$and Mw is the molecular weight of the active material.

$Q_{theoretical}$ = (1x26.801×10^3)/(0.36*308.865) mA h g^{-1}

= 241 mA h g^{-1}

LFNS

The average voltage of LTO with respect to Li metal is represented as

V = − [E(LFNS) − E(FNS) − E(Li)]/F -----Eqn. (1)

where E is the average energy of fully relaxed ground state structure, F is the Faraday constant.

V=-[((509.042)-(-298.782)-(-204.976)) eV]/(96.5 kJ/mol)

V= 5.284 V ~ 5.28 V

Single-electron oxidation voltage (V_{ox}) related to the Li^+/Li reference electrode was measured as follows:

V_{ox} (vs. Li+/Li) = [E(LFNS) − E(FNS)- E(Li)]/F+ $E_{SCE\ /SHE}$ + $E_{(Li+/Li)/SHE}$ Eqn. S19

where F is Faraday's constant. $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/Li)/SHE}$ (−3.04 V) are the potentials of an electron in a vacuum and of a metallic lithium electrode

V_{ox}(vs.Li+/Li)=[(509.042)-(-298.782)-(-204.976))]/(96.5kJ/mol)+0.24-3.04 V

V_{ox}(vs.Li+/Li) = 5.284 V +0.24-3.04 V = 2.484 V

Reduction potential is given as

V_{rx} (vs. Li^+/Li) = -[E(LFNS) − E(FNS) - E(Li)]/F + $E_{\circ(Li+/Li)/SCE}$ Eqn. S20

Where F is Faraday's constant. $E_{(Li+/Li)/SCE}$ (-3.04 V) are the potentials of metallic lithium with respect to saturated calomel electrode

V_{ox}(vs.Li+/Li)=-[(509.042)-(-298.782)-(-204.976))]/(96.5kJ/mol) - 3.04 V

V_{ox}(vs.Li+/Li) = 5.284 V - 3.04 V = -2.244 V

Average volumetric energy density is given as

$\Omega = -[E(LFNS) - E(FNS) - E(Li)]/V_{av}$

where Vav is the average volume of the fully relaxed ground state structure.

$\Omega = -$ [((509.042)-(-298.782)-(-204.976)) eV]/(192.809 $\times 10^{-24}$ cm^3)

Ω = [5.284 x1.602$\times 10^{-19}$ j]/(192.809 $\times 10^{-24}$ cm^3) [1eV=1.602$\times 10^{-19}$ j],

[one joul (J) = 2.77778e-7 kW h]

Ω = [5.071 x 1.602$\times 10^{-19}$ x 2.77778e-7 kW h]/(192.809$\times 10^{-24}$ cm^3)

Average volumetric energy density (Ω) = 1.17 W h/cm^3

Average volumetric power density = 1.17 W/cm^3

Specific energy is expressed as

$\gamma = -[E(LFNS) - E(FNS) - E(Li)]/m_{av}$ ----------(3)

where m_{av} is the average mass of a fully relaxed ground state structure

$\gamma = -[(509.042)-(-298.782)-(-204.976))$ eV]/(34.68769 g/mol)

[5.284 x96.485kj/mole]/(34.68769 g/mol)

[5.284 x96.485x2.77778 e-4 kW h]/(34.68769 g)

= 4.0827 Wh/g 1eV= 96.485kj/mole, kJ = 2.77778 e-4 kW h

Gravimetric energy density = 4.083 kWh/kg

Gravimetric power density = 4.083 kW/kg

Theoretical capacity

The theoretical capacity of a cathode material can be calculated by Faraday's law:

$Q_{theoretical} = (nF) / (3600*Mw)$ mA h g^{-1} Eqn. S21

Where n is the number of charge carriers, F is the Faraday constant $F=26.801\times10^3$ mA h mol^{-1} and Mw is the molecular weight of the active material.

$Q_{theoretical} = (1x26.801\times10^3)/(0.36*358.5404)$ mA h g^{-1}

= 207.6 mA h g^{-1}

FNS

Theoretical capacity

The theoretical capacity of a cathode material can be calculated by Faraday's law:

$Q_{theoretical} = (nF) / (3600*Mw)$ mA h g^{-1} Eqn. S21

Where n is the number of charge carriers, F is the Faraday constant $F=26.801\times10^3$ mA h mol^{-1} and Mw is the molecular weight of the active material.

$Q_{theoretical} = (1x26.801\times10^3)/(0.36*344.6584)$ mA h g^{-1}

= 216 mA h g^{-1}

Electrochemical properties of full cell

Graphite (C_6)/LFCS cell

DFT calculations of Gr/LFCS cells are given below

Average voltage of C_6/LFCS cell,

$$V = -[E(LFCS) + E(C_6) - E(LiC_6) - E(FCS)]/F \quad ---(6)[1]$$

$$V = -[(-425.6134) + (-55.261) - (-260.303) - (-215.648)\ eV]/96.5kJ/mol$$

$$V = -[-480.261\ eV + 475.951\ eV)]/96.5kJ/mol$$

$$V = -[-4.31\ eV)]/96.5kJ/mol = 4.31\ V \qquad [1eV = 96.5kJ/mol]$$

The oxidation potential of C_6/LFCS cell

V_{ox} (vs. Li+/ C_6) = [E(LFCS) − E(FCS) − E(Li)]/F+ $E_{SCE\ /SHE} - E_{(Li+/\ C6)/SHE}$ ---------- Eq. (S22)

where $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/C6)/SHE}$ (−3.0 V) are the potentials of an electron in a vacuum and of a graphite electrode [1].

V_{ox} (vs. Li^+/C_6) = [((-425.6134) - (-215.648) - (-204.976))) eV]/F+ $E_{SCE\ /SHE} - E_{(Li+/Li)/SHE}$

$$V_{ox}\ (vs.\ Li^+/C_6) = 4.9894\ V + 0.24\ V - 3.0\ V = 2.2294 \sim 2.23\ V$$

Reduction potential is given as

V_{rox} (vs. Li^+/C6) = [E(LFCS) − E(FCS) − E(Li)]/F - $E_{\circ(Li+/C6)/SCE}$ --------- (8) [1]

V_{rox} (vs.Li^+/C6)=-[(-425.6134) - (-215.648) - (-204.976))) eV]/ 96.5kJ/mol - 3.0 V

V_{rox} (vs. Li^+/ LTO) = 4.9894 V -3.0 V = 1.9894 V ~ 1.989 V

The gravimetric energy density of **C_6**/ LFCS cell

$$V = -[E(LFCS) + E(C_6) - E(LiC_6) - E(FCS)]/m_{av} \quad ----------(9)\ [1]$$

V=-[(-425.6134)+(-55.261)-(-260.303) - (-215.648) eV]/[34.39799 g/ mol

V = [4.31 eV)]/[34.39799 g/ mol

V = [4.31 x 96.485 kJ/mol)]/ 34.39799 g/ mol, [1eV = 4.45 Wh]

1eV= 96.485kj/mole, kJ = 2.77778 e-4 kW h

V = [3.99 x 96.485 kJ)]/ 34.39799 g

V = [3.99 x 96.485 x 2.77778 e-4 kW h)]/ 34.39799 g

= 3.10883 Wh/g = 3.109 Wh/g

= 3.109 kW h kg^{-1}

Gravimetrical power density of **C_6/LFCS** cell = 3.109 kW kg^{-1}

The volumetric energy density of **C_6**/ LFCS cell

$$V = -[E(LFCS) + E(C_6) - E(LiC_6) - E(FCS)]/V_{av} \text{ ----------(9) [1]}$$

$V=-[(-425.6134)+(-55.261)-(-260.303) - (-215.648)\ eV]/[\ (193.039\ \times 10^{-24}\ cm^3)$

$V = [4.9234\ eV)]/[\ (193.039\ \times 10^{-24}\ cm^3)\ ,\ )$ [1eV=1.602×10^{-19} j],

[one joul (J) = 2.77778e-7 kW h]

$V = [4.9234 \text{ x } 1.602\times 10^{-19}\ j)]/\ (193.039\ \times 10^{-24}\ cm^3)$

$V = [4.9234 \text{ x } 1.602\times 10^{-19} \text{ x } 2.77778e\text{-}7\ kW\ h\ )]/\ (193.039\ \times 10^{-24}\ cm^3)$

$V = 1.135\ W\ h\ cm^{-3}$

The volumetric energy density of **C_6/ LFCS cell** = 1.135 W h cm^{-3}

The volumetric power density of **C_6/ LFCS cell** = 1.135 W cm^{-3}

Graphite (C_6)/LFMS cell

DFT calculations of Gr/LFCS cells are given below

Average voltage of C_6/LFCS cell,

$$V= -[E(LFMS) +E(C_6)-E(LiC_6)-E(MCS)]/F \text{ ---(6)[1]}$$

$V= -[(-442.993)+(-55.261)-(-260.303) - (-232.946)\ eV]/96.5kJ/mol$
$V= -[-498.254\ eV + 493.249\ eV)]/96.5kJ/mol$
$V= -[-5.004\ eV)]/96.5kJ/mol = 5.0\ V$ [1eV = 96.5kJ/mol]

The oxidation potential of C_6/LFMS cell

V_{ox} (vs. Li+/ C_6) = [E(LFMS) − E(FMS) − E(Li)]/F+ $E_{SCE\ /SHE}$ − $E_{(Li+/\ C6)/SHE}$ ---------- Eq. (S22)
where $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/C6)/SHE}$ (−3.0 V) are the potentials of an electron in a vacuum and of a graphite electrode [1].

V_{ox} (vs. Li^+/C_6) = [((-442.993) - (-232.946) - (-204.976))) eV]/F+ $E_{SCE\ /SHE}$ − $E_{(Li+/Li)/SHE}$

V_{ox} (vs. Li^+/C_6) = 5.0710 V +0.24 V-3.0 V = 2.311 V

Reduction potential is given as

V_{rox} (vs. Li^+/C6) = [E(LFMS) − E(FMS) − E(Li)]/F - $E_{\circ(Li+/C6)/SCE}$ --------- (8) [1]
V_{rox} (vs.Li^+/C6)=-[(-442.993) - (-232.946) - (-204.976))) eV]/ 96.5kJ/mol - 3.0 V
V_{rox} (vs. Li^+/ LTO) = 5.071 V -3.0 V = 2.071 V

The gravimetric energy density of **C_6**/ LFCS cell

$$V = -[E(LFMS) + E(C_6) - E(LiC_6) - E(FMS)]/m_{av} \text{ ----------(9) [1]}$$

$V=-[(-442.993)+(-55.261)-(-260.303) - (-232.946)\ eV]/[35.00533\ g/mol$

$V= -[-498.254\ eV + 493.249\ eV)]/ 35.00533\ g/mol$

$V = [5.004\ eV)]/[35.00533\ g/mol$

$V = [5.004 \times 96.485\ kJ/mol)]/ 35.00533\ g/mol$, [1eV = 4.45 Wh]

1eV= 96.485kj/mole, kJ = 2.77778 e-4 kW h

$V = [5.004 \times 96.485\ kJ)]/ 35.00533\ g$

$V = [5.004 \times 96.485 \times 2.77778\text{ e-}4\ kW\ h)]/ 35.00533\ g$

$= 3.83125\ Wh/g = 3.831\ Wh/g$

$= 3.831\ kW\ h\ kg^{-1}$

Gravimetric energy density of **C_6**/ LFMS cell $= 3.831\ kW\ h\ kg^{-1}$

Gravimetrical power density of **C_6/LFMS** cell $= 3.831\ kW\ kg^{-1}$

The volumetric energy density of **C_6**/ LFMS cell

$$V = -[E(LFMS) + E(C_6) - E(LiC_6) - E(FMS)]/V_{av} \text{ ----------(9) [1]}$$

$V=-[(-442.993)+(-55.261)-(-260.303) - (-232.946)\ eV]/[\ (196.217\ \times 10^{-24}\ cm^3)$

$V = [5.004\ eV)]/[\ (196.217\ \times 10^{-24}\ cm^3)\ ,\ )$ [1eV=1.602×10^{-19} j],

[one joul (J) = 2.77778e-7 kW h]

$V = [5.004 \times 1.602 \times 10^{-19}\ j)]/ (196.217 \times 10^{-24}\ cm^3)$

$V = [5.004 \times 1.602 \times 10^{-19} \times 2.77778\text{e-}7\ kW\ h)]/ (196.217 \times 10^{-24}\ cm^3)$

$V = 1.14\ W\ h\ cm^{-3}$

The volumetric energy density of **C_6**/ LFMS cell $= 1.14\ W\ h\ cm^{-3}$

The volumetric power density of **C_6**/ LFMS cell $= 1.14\ W\ cm^{-3}$

Graphite (C_6)/LFNS cell

DFT calculations of Gr/LFNS cells are given below

Average voltage of C_6/LFNS cell,

$$V= -[E(LFNS) +E(C_6)-E(LiC_6)-E(FNS)]/F \quad ---(6)[1]$$

V= −[(-509.042)+(-55.261)-(-260.303) - (-298.782) eV]/96.5kJ/mol
V= −[-564.303 eV + 559.085 eV)]/96.5kJ/mol
V= −[-5.218 eV)]/96.5kJ/mol = 5.218 V [1eV = 96.5kJ/mol]

The oxidation potential of C_6/LFMS cell

V_{ox} (vs. Li+/ C_6) = [E(LFNS) − E(FNS) − E(Li)]/F+ $E_{SCE\ /SHE}$ − $E_{(Li+/\ C6)/SHE}$ ---------- Eq. (S22)
where $E_{\circ\ SCE\ /SHE}$ (0.24) and $E_{\circ(Li+/C6)/SHE}$ (−3.0 V) are the potentials of an electron in a vacuum and of a graphite electrode [1].

V_{ox} (vs. Li^+/C_6) = [((-509.042) - (-298.782) - (-204.976))) eV]/F+ $E_{SCE\ /SHE}$ − $E_{(Li+/Li)/SHE}$

V_{ox} (vs. Li^+/C_6) = 5.284 V +0.24 V-3.0 V = 2.524 V

Reduction potential is given as

V_{rox} (vs. Li^+/C6) = [E(LFNS) − E(FNS) − E(Li)]/F - $E_{\circ(Li+/C6)/SCE}$ --------- (8) [1]
V_{rox} (vs.Li^+/C6)=-[(-509.042) - (-298.782) - (-204.976))) eV]/ 96.5kJ/mol - 3.0 V
V_{rox} (vs. Li^+/ LTO) = 5.284 V -3.0 V = 2.284 V

The gravimetric energy density of **C_6**/ LFNS cell

V = -[E(LFNS) + E(C_6) - E(LiC_6) - E(FNS)]/m_{av} ----------(9) [1]

V=-[(-509.042)+(-55.261)-(-260.303) - (-298.782) eV]/[34.68769 g/ mol

V= −[-564.303 eV + 559.085 eV)]/ 34.68769 g/ mol
V = [5.218 eV)]/[34.68769 g/ mol
V = [5.218 x 96.485 kJ/mol)]/ 34.68769 g/ mol, [1eV = 4.45 Wh]

1eV= 96.485kj/mole, kJ = 2.77778 e-4 kW h

V = [5.218 x 96.485 kJ)]/ 34.68769 g
V = [5.218 x 96.485 x 2.77778 e-4 kW h)]/ 34.68769 g

= 4.03168 Wh/g = 4.032 Wh/g

= 4.032 kW h kg^{-1}

Gravimetric energy density of **C_6**/ LFNS cell = 4.032 kW h kg^{-1}
Gravimetrical power density of **C_6/LFNS** cell = 4.032 kW kg^{-1}

The volumetric energy density of **C_6**/ LFNS cell

V = -[E(LFNS) + E(C_6) - E(LiC_6) - E(FNS)]/V_{av} ----------(9) [1]

V=-[(-509.042)+(-55.261)-(-260.303) - (-298.782) eV]/[(192.809 $\times 10^{-24}$ cm^3)

V = [5.218 eV)]/[(192.809 $\times 10^{-24}$ cm^3) ,) [1eV=1.602$\times 10^{-19}$ j],

[one joul (J) = 2.77778e-7 kW h]

V = [5.218 x 1.602$\times 10^{-19}$ j)]/ (192.809 $\times 10^{-24}$ cm^3)

V = [5.218 x 1.602$\times 10^{-19}$ x 2.77778e-7 kW h)]/ (192.809 $\times 10^{-24}$ cm^3)

V = 1.204 W h cm^{-3}

The volumetric energy density of C_6/ LFNS cell = 1.204 W h cm^{-3}

The volumetric power density of C_6/ LFNS cell = 1.204 W cm^{-3}

```
OpenGL version: 4.6.14802 Compatibility Profile Context 21.40.56.05 30.0.14056.5001
Video configuration: AMD Radeon(TM) Graphics
Maximum supported width and height of the viewport: 16384 x 16384
OpenGL depth buffer bit: 16


C:\simulation\DFT Li-ion battery simulation\Tevorite and triplets\L2FeCSF P1.cif
================================================================================
=
Title               f2 fe2 li4 o8 p2

Lattice type        P
Space group name    P 1
Space group number  1
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 5.45338  7.51205  5.33977 108.6064  95.8897 107.3919

Unit-cell volume = 193.039384 Å^3

Structure parameters

                       x          y          z          Occ.     B     Site
Sym.
   1 F   1          -0.89171   -0.26468    0.82970    1.000    1.000    1a
1
   2 F   2          -0.10752   -0.73232    0.18037    1.000    1.000    1a
1
   3 Co  3          -0.99868   -0.00823    0.98778    1.000    1.000    1a
1
   4 Fe  4          -0.00157   -0.49174    0.99646    1.000    1.000    1a
1
   5 Li  5          -0.91903   -0.46876    0.50169    1.000    1.000    1a
1
   6 Li  6          -0.54676   -0.10386    0.83505    1.000    1.000    1a
1
```

```
   7 Li   7          -0.43472   -0.68054    0.23784    1.000    1.000    1a
1
   8 Li   8          -0.16783   -0.85123    0.47638    1.000    1.000    1a
1
   9 O    9          -0.80386   -0.62306    0.71349    1.000    1.000    1a
1
  10 O   10          -0.66549   -0.36169    0.31276    1.000    1.000    1a
1
  11 O   11          -0.75764   -0.91544    0.36206    1.000    1.000    1a
1
  12 O   12          -0.64831   -0.86330    0.86891    1.000    1.000    1a
1
  13 O   13          -0.25679   -0.08275    0.62266    1.000    1.000    1a
1
  14 O   14          -0.33708   -0.13248    0.13453    1.000    1.000    1a
1
  15 O   15          -0.34512   -0.65109    0.66110    1.000    1.000    1a
1
  16 O   16          -0.22826   -0.40258    0.27218    1.000    1.000    1a
1
  17 S   17          -0.63932   -0.76288    0.65458    1.000    1.000    1a
1
  18 S   18          -0.37183   -0.24824    0.33021    1.000    1.000    1a
1
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
35 atoms, 40 bonds, 8 polyhedra; CPU time = 4 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

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35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms
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35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

```
================================================================================
=
Title               f2 fe2 li4 o8 p2

Lattice type        P
Space group name    P 1
Space group number  1
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 5.45338  7.51205  5.33977 108.6064  95.8897 107.3919

Unit-cell volume = 193.039384 Å^3

Structure parameters

                       x          y          z          Occ.     B    Site
Sym.
   1 F   1          -0.89171   -0.26468    0.82970    1.000    1.000    1a
1
   2 F   2          -0.10752   -0.73232    0.18037    1.000    1.000    1a
1
   3 Co  3          -0.99868   -0.00823    0.98778    1.000    1.000    1a
1
   4 Fe  4          -0.00157   -0.49174    0.99646    1.000    1.000    1a
1
   5 Li  5          -0.91903   -0.46876    0.50169    1.000    1.000    1a
1
   6 Li  6          -0.54676   -0.10386    0.83505    1.000    1.000    1a
1
   7 Li  7          -0.43472   -0.68054    0.23784    1.000    1.000    1a
1
   8 Li  8          -0.16783   -0.85123    0.47638    1.000    1.000    1a
1
   9 O   9          -0.80386   -0.62306    0.71349    1.000    1.000    1a
1
  10 O   10         -0.66549   -0.36169    0.31276    1.000    1.000    1a
1
  11 O   11         -0.75764   -0.91544    0.36206    1.000    1.000    1a
1
  12 O   12         -0.64831   -0.86330    0.86891    1.000    1.000    1a
1
  13 O   13         -0.25679   -0.08275    0.62266    1.000    1.000    1a
1
  14 O   14         -0.33708   -0.13248    0.13453    1.000    1.000    1a
1
  15 O   15         -0.34512   -0.65109    0.66110    1.000    1.000    1a
1
  16 O   16         -0.22826   -0.40258    0.27218    1.000    1.000    1a
1
  17 S   17         -0.63932   -0.76288    0.65458    1.000    1.000    1a
1
  18 S   18         -0.37183   -0.24824    0.33021    1.000    1.000    1a
1
================================================================================
=

Number of polygons and unique vertices on isosurface = 0 (0)
```

35 atoms, 40 bonds, 8 polyhedra; CPU time = 2 ms

Atom: 5   5 Li   0.08097   0.53124   0.50169 (1, 1, 0)+ x, y, z
          (x,y,z): -1.02618   2.82646   2.47731
              Occ. = 1.000   B = 1.00000   1a   1

POLYHEDRON:

5	5	Li	0.08097	0.53124	0.50169	(1, 1, 0)+ x, y, z
1	1	F	0.10829	0.73532	0.82970	(1, 1, 0)+ x, y, z
2	2	F	-0.10752	0.26768	0.18037	(0, 1, 0)+ x, y, z
16	16	O	-0.22826	0.59742	0.27218	(0, 1, 0)+ x, y, z
9	9	O	0.19614	0.37694	0.71349	(1, 1, 0)+ x, y, z
10	10	O	0.33451	0.63831	0.31276	(1, 1, 0)+ x, y, z

l(5-1) = 1.88060(0) Å
l(5-2) = 2.04305(0) Å
l(5-16) = 2.24915(0) Å
l(5-9) = 2.03545(0) Å
l(5-10) = 1.92760(0) Å

Average bond length = 2.0272 Å
Polyhedral volume = 6.2448 Å^3
Distortion index (bond length) = 0.04857
Effective coordination number = 4.2416

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
1	1	F	0.10829	0.73532	0.82970	-0.298	-0.446	-1.000
2	2	F	-0.10752	0.26768	0.18037	-0.182	0.056	-1.000
16	16	O	-0.22826	0.59742	0.27218	-0.068	0.266	-2.000
9	9	O	0.19614	0.37694	0.71349	-0.187	0.305	-2.000
10	10	O	0.33451	0.63831	0.31276	-0.264	0.209	-2.000
5	5	Li	0.08097	0.53124	0.50169		6.866	-1.000

POLYHEDRON:

6	6	Li	0.45324	0.89614	0.83505	(1, 1, 0)+ x, y, z
1	1	F	0.10829	0.73532	0.82970	(1, 1, 0)+ x, y, z
14	14	O	0.66292	0.86752	1.13453	(1, 1, 1)+ x, y, z
12	12	O	0.35169	1.13670	0.86891	(1, 2, 0)+ x, y, z
13	13	O	0.74321	0.91725	0.62266	(1, 1, 0)+ x, y, z

l(6-1) = 1.89931(0) Å
l(6-14) = 1.97538(0) Å
l(6-12) = 2.00382(0) Å
l(6-13) = 2.03589(0) Å

Average bond length = 1.9786 Å
Polyhedral volume = 3.3550 Å^3
Distortion index (bond length) = 0.02085
Quadratic elongation = 1.1205
Bond angle variance = 399.4172 deg.^2
Effective coordination number = 3.8870

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion

q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
1	1	F	0.10829	0.73532	0.82970	-0.312	-0.446	-1.000
14	14	O	0.66292	0.86752	1.13453	-0.252	0.436	-2.000
12	12	O	0.35169	1.13670	0.86891	-0.230	0.528	-2.000
13	13	O	0.74321	0.91725	0.62266	-0.206	0.306	-2.000
6	6	Li	0.45324	0.89614	0.83505		2.674	-1.000

POLYHEDRON:

3	3	Co	0.00132	0.99177	0.98778	(1, 1, 0)+ x, y, z

1	1	F	0.10829	0.73532	0.82970	(1, 1, 0)+ x, y, z
14	14	O	-0.33708	0.86752	1.13453	(0, 1, 1)+ x, y, z
13	13	O	-0.25679	0.91725	0.62266	(0, 1, 0)+ x, y, z
2	2	F	-0.10752	1.26768	1.18037	(0, 2, 1)+ x, y, z
11	11	O	0.24236	1.08456	1.36206	(1, 2, 1)+ x, y, z
12	12	O	0.35169	1.13670	0.86891	(1, 2, 0)+ x, y, z

l(3-1) = 2.12115(0) Å
l(3-14) = 2.15049(0) Å
l(3-13) = 2.08928(0) Å
l(3-2) = 2.28173(0) Å
l(3-11) = 2.05722(0) Å
l(3-12) = 2.16455(0) Å

Average bond length = 2.1441 Å
Polyhedral volume = 12.8999 Å^3
Distortion index (bond length) = 0.02558
Quadratic elongation = 1.0136
Bond angle variance = 41.1500 deg.^2
Effective coordination number = 5.7447

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
1	1	F	0.10829	0.73532	0.82970	0.531	-0.446	-1.000
14	14	O	-0.33708	0.86752	1.13453	0.488	0.436	-2.000
13	13	O	-0.25679	0.91725	0.62266	0.578	0.306	-2.000
2	2	F	-0.10752	1.26768	1.18037	0.309	0.056	-1.000
11	11	O	0.24236	1.08456	1.36206	0.626	-0.036	-2.000
12	12	O	0.35169	1.13670	0.86891	0.468	0.528	-2.000
3	3	Co	0.00132	0.99177	0.98778	22.777	3.000	

POLYHEDRON:

18	18	S	0.62817	0.75176	0.33021	(1, 1, 0)+ x, y, z

10	10	O	0.33451	0.63831	0.31276	(1, 1, 0)+ x, y, z
13	13	O	0.74321	0.91725	0.62266	(1, 1, 0)+ x, y, z
14	14	O	0.66292	0.86752	0.13453	(1, 1, 0)+ x, y, z
16	16	O	0.77174	0.59742	0.27218	(1, 1, 0)+ x, y, z

l(18-10) = 1.54997(0) Å
l(18-13) = 1.57212(0) Å
l(18-14) = 1.55108(0) Å
l(18-16) = 1.55449(0) Å

Average bond length = 1.5569 Å

Polyhedral volume = 1.9310 Å^3
Distortion index (bond length) = 0.00488
Quadratic elongation = 1.0020
Bond angle variance = 8.0514 deg.^2
Effective coordination number = 3.9956

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
10	10	O	0.33451	0.63831	0.31276	-0.513	0.209	-2.000
13	13	O	0.74321	0.91725	0.62266	-0.471	0.306	-2.000
14	14	O	0.66292	0.86752	0.13453	-0.511	0.436	-2.000
16	16	O	0.77174	0.59742	0.27218	-0.505	0.266	-2.000
18	18	S	0.62817	0.75176	0.33021		14.125	-2.000

POLYHEDRON:

17	17	S	0.36068	0.23712	0.65458	(1, 1, 0)+ x, y, z		
9	9	O	0.19614	0.37694	0.71349	(1, 1, 0)+ x, y, z		
11	11	O	0.24236	0.08456	0.36206	(1, 1, 0)+ x, y, z		
12	12	O	0.35169	0.13670	0.86891	(1, 1, 0)+ x, y, z		
15	15	O	0.65488	0.34891	0.66110	(1, 1, 0)+ x, y, z		

l(17-9) = 1.55493(0) Å
l(17-11) = 1.54218(0) Å
l(17-12) = 1.55615(0) Å
l(17-15) = 1.56362(0) Å

Average bond length = 1.5542 Å
Polyhedral volume = 1.9189 Å^3
Distortion index (bond length) = 0.00387
Quadratic elongation = 1.0027
Bond angle variance = 10.2212 deg.^2
Effective coordination number = 3.9966

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
9	9	O	0.19614	0.37694	0.71349	-0.499	0.305	-2.000
11	11	O	0.24236	0.08456	0.36206	-0.523	-0.036	-2.000
12	12	O	0.35169	0.13670	0.86891	-0.496	0.528	-2.000
15	15	O	0.65488	0.34891	0.66110	-0.482	0.376	-2.000
17	17	S	0.36068	0.23712	0.65458		-21.485	-2.000

POLYHEDRON:

4	4	Fe	0.99843	0.50826	0.99646	(1, 1, 0)+ x, y, z		
15	15	O	0.65488	0.34891	0.66110	(1, 1, 0)+ x, y, z		
2	2	F	0.89248	0.26768	1.18037	(1, 1, 1)+ x, y, z		
16	16	O	0.77174	0.59742	1.27218	(1, 1, 1)+ x, y, z		
9	9	O	1.19614	0.37694	0.71349	(2, 1, 0)+ x, y, z		
1	1	F	1.10829	0.73532	0.82970	(2, 1, 0)+ x, y, z		
10	10	O	1.33451	0.63831	1.31276	(2, 1, 1)+ x, y, z		

l(4-15) = 2.18004(0) Å
l(4-2) = 2.27797(0) Å
l(4-16) = 2.09373(0) Å
l(4-9) = 2.10660(0) Å
l(4-1) = 2.12815(0) Å
l(4-10) = 2.09940(0) Å

Average bond length = 2.1476 Å
Polyhedral volume = 12.8251 Å^3
Distortion index (bond length) = 0.02525
Quadratic elongation = 1.0207
Bond angle variance = 69.1779 deg.^2
Effective coordination number = 5.8087

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
15	15	O	0.65488	0.34891	0.66110	0.451	0.376	-2.000
2	2	F	0.89248	0.26768	1.18037	0.321	0.056	-1.000
16	16	O	0.77174	0.59742	1.27218	0.576	0.266	-2.000
9	9	O	1.19614	0.37694	0.71349	0.557	0.305	-2.000
1	1	F	1.10829	0.73532	0.82970	0.526	-0.446	-1.000
10	10	O	1.33451	0.63831	1.31276	0.568	0.209	-2.000
4	4	Fe	0.99843	0.50826	0.99646	-20.391	3.000	

POLYHEDRON:

8	8	Li	0.83217	0.14877	0.47638	(1, 1, 0)+ x, y, z
2	2	F	0.89248	0.26768	0.18037	(1, 1, 0)+ x, y, z
14	14	O	0.66292	-0.13248	0.13453	(1, 0, 0)+ x, y, z
15	15	O	0.65488	0.34891	0.66110	(1, 1, 0)+ x, y, z
13	13	O	0.74321	-0.08275	0.62266	(1, 0, 0)+ x, y, z
11	11	O	1.24236	0.08456	0.36206	(2, 1, 0)+ x, y, z
9	9	O	1.19614	0.37694	0.71349	(2, 1, 0)+ x, y, z

l(8-2) = 2.05828(0) Å
l(8-14) = 2.16222(0) Å
l(8-15) = 2.07037(0) Å
l(8-13) = 2.07618(0) Å
l(8-11) = 2.51922(0) Å
l(8-9) = 2.13218(0) Å

Average bond length = 2.1697 Å
Polyhedral volume = 11.9004 Å^3
Distortion index (bond length) = 0.05369
Quadratic elongation = 1.1001
Bond angle variance = 326.2867 deg.^2
Effective coordination number = 5.2014

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
2	2	F	0.89248	0.26768	0.18037	-0.217	0.056	-1.000
14	14	O	0.66292	-0.13248	0.13453	-0.161	0.436	-2.000
15	15	O	0.65488	0.34891	0.66110	-0.211	0.376	-2.000
13	13	O	0.74321	-0.08275	0.62266	-0.207	0.306	-2.000
11	11	O	1.24236	0.08456	0.36206	-0.027	-0.036	-2.000

```
   9       9  O  1.19614  0.37694  0.71349   -0.177  0.305 -2.000
-------------------------------------------------------------------------------
   8       8 Li  0.83217  0.14877  0.47638           6.745 -1.000


POLYHEDRON:
   7       7 Li  0.56528  0.31946  0.23784  ( 1, 1, 0)+ x, y, z
-------------------------------------------------------------------------------
   2       2  F  0.89248  0.26768  0.18037  ( 1, 1, 0)+ x, y, z
  11      11  O  0.24236  0.08456  0.36206  ( 1, 1, 0)+ x, y, z
  12      12  O  0.35169  0.13670 -0.13109  ( 1, 1,-1)+ x, y, z
  15      15  O  0.65488  0.34891  0.66110  ( 1, 1, 0)+ x, y, z
  16      16  O  0.77174  0.59742  0.27218  ( 1, 1, 0)+ x, y, z
-------------------------------------------------------------------------------

l(7-2) =  1.96990(0) Å
l(7-11) =  2.40496(0) Å
l(7-12) =  1.99241(0) Å
l(7-15) =  2.18757(0) Å
l(7-16) =  1.99226(0) Å
---------------------------------------
Average bond length =  2.1094 Å
Polyhedral volume =  6.5179 Å^3
Distortion index (bond length) = 0.07086
Effective coordination number =  4.0385

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
   2       2  F  0.89248  0.26768  0.18037   -0.286  0.056 -1.000
  11      11  O  0.24236  0.08456  0.36206   -0.040 -0.036 -2.000
  12      12  O  0.35169  0.13670 -0.13109   -0.269  0.528 -2.000
  15      15  O  0.65488  0.34891  0.66110   -0.135  0.376 -2.000
  16      16  O  0.77174  0.59742  0.27218   -0.269  0.266 -2.000
-------------------------------------------------------------------------------
   7       7 Li  0.56528  0.31946  0.23784           6.690 -1.000


POLYHEDRON:
   7       7 Li  0.56528  0.31946  0.23784  ( 1, 1, 0)+ x, y, z
-------------------------------------------------------------------------------
   2       2  F  0.89248  0.26768  0.18037  ( 1, 1, 0)+ x, y, z
  11      11  O  0.24236  0.08456  0.36206  ( 1, 1, 0)+ x, y, z
  12      12  O  0.35169  0.13670 -0.13109  ( 1, 1,-1)+ x, y, z
  15      15  O  0.65488  0.34891  0.66110  ( 1, 1, 0)+ x, y, z
  16      16  O  0.77174  0.59742  0.27218  ( 1, 1, 0)+ x, y, z
-------------------------------------------------------------------------------

l(7-2) =  1.96990(0) Å
l(7-11) =  2.40496(0) Å
l(7-12) =  1.99241(0) Å
l(7-15) =  2.18757(0) Å
l(7-16) =  1.99226(0) Å
---------------------------------------
Average bond length =  2.1094 Å
Polyhedral volume =  6.5179 Å^3
Distortion index (bond length) = 0.07086
Effective coordination number =  4.0385

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
```

```
------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
   2       2  F  0.89248  0.26768  0.18037   -0.286  0.056 -1.000
  11      11  O  0.24236  0.08456  0.36206   -0.040 -0.036 -2.000
  12      12  O  0.35169  0.13670 -0.13109   -0.269  0.528 -2.000
  15      15  O  0.65488  0.34891  0.66110   -0.135  0.376 -2.000
  16      16  O  0.77174  0.59742  0.27218   -0.269  0.266 -2.000
------------------------------------------------------------------------------
   7       7 Li  0.56528  0.31946  0.23784           6.690 -1.000


POLYHEDRON:
  17      17  S  0.36068  0.23712  0.65458  ( 1, 1, 0)+ x, y, z
------------------------------------------------------------------------------
   9       9  O  0.19614  0.37694  0.71349  ( 1, 1, 0)+ x, y, z
  11      11  O  0.24236  0.08456  0.36206  ( 1, 1, 0)+ x, y, z
  12      12  O  0.35169  0.13670  0.86891  ( 1, 1, 0)+ x, y, z
  15      15  O  0.65488  0.34891  0.66110  ( 1, 1, 0)+ x, y, z
------------------------------------------------------------------------------

l(17-9) =  1.55493(0) Å
l(17-11) =  1.54218(0) Å
l(17-12) =  1.55615(0) Å
l(17-15) =  1.56362(0) Å
--------------------------------------
Average bond length =  1.5542 Å
Polyhedral volume =  1.9189 Å^3
Distortion index (bond length) = 0.00387
Quadratic elongation =  1.0027
Bond angle variance =  10.2212 deg.^2
Effective coordination number =  3.9966

Charge distribution
------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
   9       9  O  0.19614  0.37694  0.71349   -0.499  0.305 -2.000
  11      11  O  0.24236  0.08456  0.36206   -0.523 -0.036 -2.000
  12      12  O  0.35169  0.13670  0.86891   -0.496  0.528 -2.000
  15      15  O  0.65488  0.34891  0.66110   -0.482  0.376 -2.000
------------------------------------------------------------------------------
  17      17  S  0.36068  0.23712  0.65458          -21.485 -2.000



OpenGL version: 4.6.14802 Compatibility Profile Context 21.40.56.05 30.0.14056.5001
Video configuration: AMD Radeon(TM) Graphics
Maximum supported width and height of the viewport: 16384 x 16384
OpenGL depth buffer bit: 16


C:\simulation\DFT Li-ion battery simulation\Tevorite and triplets\LiFeMSF_triclinic
P-12.cif
================================================================================
=
Title               li2 fe2 s2 o8 f2

Lattice type        P
Space group name    P 1
Space group number  1
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
```

5.25236 5.59647 7.40296 107.2483 107.2924 97.0660

Unit-cell volume = 193.034809 Å^3

Structure parameters

			x	y	z	Occ.	B	Site Sym.
1	Li	Li0	0.26371	0.62117	0.78646	1.000	1.000	1a 1
2	Li	Li1	0.73628	0.37883	0.21354	1.000	1.000	1a 1
3	Mn	Mn2	0.00000	0.00000	0.50000	1.000	1.000	1a 1
4	Fe	Fe3	0.00000	0.00000	0.00000	1.000	1.000	1a 1
5	S	S4	0.32506	0.63233	0.24455	1.000	1.000	1a 1
6	S	S5	0.67494	0.36767	0.75545	1.000	1.000	1a 1
7	O	O6	0.59941	0.75290	0.40145	1.000	1.000	1a 1
8	O	O7	0.40060	0.24710	0.59855	1.000	1.000	1a 1
9	O	O8	0.10599	0.65088	0.33604	1.000	1.000	1a 1
10	O	O9	0.89401	0.34912	0.66396	1.000	1.000	1a 1
11	O	O10	0.32471	0.35557	0.14868	1.000	1.000	1a 1
12	O	O11	0.67529	0.64443	0.85132	1.000	1.000	1a 1
13	O	O12	0.27202	0.75515	0.08759	1.000	1.000	1a 1
14	O	O13	0.72798	0.24485	0.91241	1.000	1.000	1a 1
15	F	F14	0.11723	0.90825	0.75450	1.000	1.000	1a 1
16	F	F15	0.88276	0.09175	0.24550	1.000	1.000	1a 1

==========

Number of polygons and unique vertices on isosurface = 0 (0)
80 atoms, 90 bonds, 16 polyhedra; CPU time = 15 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms

```
================================================================================
=
Title               li2 fe2 s2 o8 f2

Lattice type        P
Space group name    P 1
Space group number  1
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 5.25236  5.59647  7.40296 107.2483 107.2924  97.0660

Unit-cell volume = 193.034809 Å^3

Structure parameters

                       x          y          z          Occ.     B    Site
Sym.
   1 Li  Li0          0.26371    0.62117    0.78646    1.000    1.000    1a
1
   2 Li  Li1          0.73628    0.37883    0.21354    1.000    1.000    1a
1
   3 Mn  Mn2          0.00000    0.00000    0.50000    1.000    1.000    1a
1
   4 Fe  Fe3          0.00000    0.00000    0.00000    1.000    1.000    1a
1
   5 S   S4           0.32506    0.63233    0.24455    1.000    1.000    1a
1
   6 S   S5           0.67494    0.36767    0.75545    1.000    1.000    1a
1
   7 O   O6           0.59941    0.75290    0.40145    1.000    1.000    1a
1
   8 O   O7           0.40060    0.24710    0.59855    1.000    1.000    1a
1
   9 O   O8           0.10599    0.65088    0.33604    1.000    1.000    1a
1
  10 O   O9           0.89401    0.34912    0.66396    1.000    1.000    1a
1
  11 O   O10          0.32471    0.35557    0.14868    1.000    1.000    1a
1
  12 O   O11          0.67529    0.64443    0.85132    1.000    1.000    1a
1
  13 O   O12          0.27202    0.75515    0.08759    1.000    1.000    1a
1
  14 O   O13          0.72798    0.24485    0.91241    1.000    1.000    1a
1
  15 F   F14          0.11723    0.90825    0.75450    1.000    1.000    1a
1
  16 F   F15          0.88276    0.09175    0.24550    1.000    1.000    1a
1
================================================================================
=
```

```
Number of polygons and unique vertices on isosurface = 0 (0)
80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms


POLYHEDRON:
   4     Fe3 Fe  0.00000  1.00000  0.00000  ( 0, 1, 0)+ x, y, z
--------------------------------------------------------------------------------
  12     O11  O -0.32471  0.64443 -0.14868  (-1, 0,-1)+ x, y, z
  14     O13  O -0.27202  1.24485 -0.08759  (-1, 1,-1)+ x, y, z
  16     F15  F -0.11724  1.09175  0.24550  (-1, 1, 0)+ x, y, z
  15     F14  F  0.11723  0.90825 -0.24550  ( 0, 0,-1)+ x, y, z
  13     O12  O  0.27202  0.75515  0.08759  ( 0, 0, 0)+ x, y, z
  11     O10  O  0.32471  1.35557  0.14868  ( 0, 1, 0)+ x, y, z
--------------------------------------------------------------------------------

l(Fe3-O11) =  2.19775(0) Å
l(Fe3-O13) =  2.19029(0) Å
l(Fe3-F15) =  2.03357(0) Å
l(Fe3-F14) =  2.03356(0) Å
l(Fe3-O12) =  2.19029(0) Å
l(Fe3-O10) =  2.19775(0) Å
---------------------------------------
Average bond length =  2.1405 Å
Polyhedral volume = 12.8898 Å^3
Distortion index (bond length) = 0.03332
Quadratic elongation =  1.0109
Bond angle variance =  29.9662 deg.^2
Effective coordination number =  5.6508

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
  12     O11  O -0.32471  0.64443 -0.14868    0.415  0.304 -2.000
  14     O13  O -0.27202  1.24485 -0.08759    0.425  0.258 -2.000
  16     F15  F -0.11724  1.09175  0.24550    0.660 -0.958 -1.000
  15     F14  F  0.11723  0.90825 -0.24550    0.660 -0.958 -1.000
  13     O12  O  0.27202  0.75515  0.08759    0.425  0.258 -2.000
  11     O10  O  0.32471  1.35557  0.14868    0.415  0.304 -2.000
--------------------------------------------------------------------------------
   4     Fe3 Fe  0.00000  1.00000  0.00000          -10.662  3.000

Input a bond valence parameter: 3.000000
Bond valence of O11: -8.74286
Bond valence of O13: -8.92087
Bond valence of F15: -13.626
Bond valence of F14: -13.6261
Bond valence of O12: -8.92087
Bond valence of O10: -8.74286
Bond valence sum =62.580
Oxidation state of the cation: +3
Expected bond length = 3.256 Å

POLYHEDRON:
   3     Mn2 Mn -0.00000  1.00000  0.50000  ( 0, 1, 0)+ x, y, z
--------------------------------------------------------------------------------
   7      O6  O -0.40059  0.75290  0.40145  (-1, 0, 0)+ x, y, z
  16     F15  F -0.11724  1.09175  0.24550  (-1, 1, 0)+ x, y, z
  10      O9  O -0.10599  1.34912  0.66396  (-1, 1, 0)+ x, y, z
   9      O8  O  0.10599  0.65088  0.33604  ( 0, 0, 0)+ x, y, z
  15     F14  F  0.11723  0.90825  0.75450  ( 0, 0, 0)+ x, y, z
   8      O7  O  0.40060  1.24710  0.59855  ( 0, 1, 0)+ x, y, z
--------------------------------------------------------------------------------
```

```
l(Mn2-O6) =  2.15521(0) Å
l(Mn2-F15) =  2.03824(0) Å
l(Mn2-O9) =  2.20535(0) Å
l(Mn2-O8) =  2.20535(0) Å
l(Mn2-F14) =  2.03824(0) Å
l(Mn2-O7) =  2.15521(0) Å
---------------------------------------
Average bond length =  2.1329 Å
Polyhedral volume = 12.8586 Å^3
Distortion index (bond length) = 0.02960
Quadratic elongation =  1.0052
Bond angle variance =  10.7819 deg.^2
Effective coordination number =  5.7154

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
   7      O6  O -0.40059  0.75290  0.40145    0.465  0.090 -2.000
  16     F15  F -0.11724  1.09175  0.24550    0.640 -0.958 -1.000
  10      O9  O -0.10599  1.34912  0.66396    0.394  0.306 -2.000
   9      O8  O  0.10599  0.65088  0.33604    0.394  0.306 -2.000
  15     F14  F  0.11723  0.90825  0.75450    0.640 -0.958 -1.000
   8      O7  O  0.40060  1.24710  0.59855    0.465  0.090 -2.000
-------------------------------------------------------------------------------
   3     Mn2 Mn -0.00000  1.00000  0.50000          -24.548  3.000

Input a bond valence parameter: 3.000000
Bond valence of O6: -9.80817
Bond valence of F15: -13.455
Bond valence of O9: -8.56521
Bond valence of O8: -8.56521
Bond valence of F14: -13.455
Bond valence of O7: -9.80806
Bond valence sum =63.657
Oxidation state of the cation: +3
Expected bond length = 3.256 Å

POLYHEDRON:
   2     Li1 Li  0.73628  0.37883  0.21354  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------
  11     O10  O  0.32471  0.35557  0.14868  ( 0, 0, 0)+ x, y, z
  14     O13  O  0.72798  0.24485 -0.08759  ( 0, 0,-1)+ x, y, z
  16     F15  F  0.88276  0.09175  0.24550  ( 0, 0, 0)+ x, y, z
   7      O6  O  0.59941  0.75290  0.40145  ( 0, 0, 0)+ x, y, z
   9      O8  O  1.10599  0.65088  0.33604  ( 1, 0, 0)+ x, y, z
-------------------------------------------------------------------------------

l(Li1-O10) =  2.04872(0) Å
l(Li1-O13) =  2.11578(0) Å
l(Li1-F15) =  1.91062(0) Å
l(Li1-O6) =  2.46424(0) Å
l(Li1-O8) =  2.07800(0) Å
---------------------------------------
Average bond length =  2.1235 Å
Polyhedral volume =  6.9062 Å^3
Distortion index (bond length) = 0.06419
Effective coordination number =  3.8579

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
```

```
                  x        y        z      delta_q    Q      q
  11     O10  O  0.32471  0.35557  0.14868   -0.235  0.304 -2.000
  14     O13  O  0.72798  0.24485 -0.08759   -0.186  0.258 -2.000
  16     F15  F  0.88276  0.09175  0.24550   -0.342 -0.958 -1.000
   7      O6  O  0.59941  0.75290  0.40145   -0.025  0.090 -2.000
   9      O8  O  1.10599  0.65088  0.33604   -0.213  0.306 -2.000
-------------------------------------------------------------------------------
   2     Li1 Li  0.73628  0.37883  0.21354           4.575 -1.000

Input a bond valence parameter: -1.000000
Bond valence of O10: -0.000263943
Bond valence of O13: -0.000220188
Bond valence of F15: -0.000383362
Bond valence of O6: -8.58579e-05
Bond valence of O8: -0.000243861
Bond valence sum = 0.001
Oxidation state of the cation: -1
Expected bond length =-1.#IO Å

POLYHEDRON:
   5      S4  S  0.32506  0.63233  0.24455  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------
  11     O10  O  0.32471  0.35557  0.14868  ( 0, 0, 0)+ x, y, z
   9      O8  O  0.10599  0.65088  0.33604  ( 0, 0, 0)+ x, y, z
  13     O12  O  0.27202  0.75515  0.08759  ( 0, 0, 0)+ x, y, z
   7      O6  O  0.59941  0.75290  0.40145  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------

l(S4-O10) =  1.49983(0) Å
l(S4-O8) =  1.49815(0) Å
l(S4-O12) =  1.49282(0) Å
l(S4-O6) =  1.47708(0) Å
---------------------------------------
Average bond length =  1.4920 Å
Polyhedral volume =  1.7023 Å^3
Distortion index (bond length) = 0.00499
Quadratic elongation =  1.0009
Bond angle variance =   3.1994 deg.^2
Effective coordination number =  3.9949

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
  11     O10  O  0.32471  0.35557  0.14868   -0.484  0.304 -2.000
   9      O8  O  0.10599  0.65088  0.33604   -0.488  0.306 -2.000
  13     O12  O  0.27202  0.75515  0.08759   -0.498  0.258 -2.000
   7      O6  O  0.59941  0.75290  0.40145   -0.530  0.090 -2.000
-------------------------------------------------------------------------------
   5      S4  S  0.32506  0.63233  0.24455          22.031 -2.000

Input a bond valence parameter: -2.000000
Bond valence of O10: -7.79852e-05
Bond valence of O8: -7.83388e-05
Bond valence of O12: -7.94752e-05
Bond valence of O6: -8.29291e-05
Bond valence sum = 0.000
Oxidation state of the cation: -2
Expected bond length =-1.#IO Å

POLYHEDRON:
   4     Fe3 Fe  0.00000  0.00000  0.00000  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------
  12     O11  O -0.32471 -0.35557 -0.14868  (-1,-1,-1)+ x, y, z
  14     O13  O -0.27202  0.24485 -0.08759  (-1, 0,-1)+ x, y, z
```

```
  16     F15  F -0.11724  0.09175  0.24550  (-1, 0, 0)+ x, y, z
  15     F14  F  0.11723 -0.09175 -0.24550  ( 0,-1,-1)+ x, y, z
  13     O12  O  0.27202 -0.24485  0.08759  ( 0,-1, 0)+ x, y, z
  11     O10  O  0.32471  0.35557  0.14868  ( 0, 0, 0)+ x, y, z
--------------------------------------------------------------------------------

l(Fe3-O11) =  2.19775(0) Å
l(Fe3-O13) =  2.19029(0) Å
l(Fe3-F15) =  2.03357(0) Å
l(Fe3-F14) =  2.03356(0) Å
l(Fe3-O12) =  2.19029(0) Å
l(Fe3-O10) =  2.19775(0) Å
---------------------------------------
Average bond length =  2.1405 Å
Polyhedral volume = 12.8898 Å^3
Distortion index (bond length) = 0.03332
Quadratic elongation =  1.0109
Bond angle variance =  29.9662 deg.^2
Effective coordination number =  5.6508

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
  12     O11  O -0.32471 -0.35557 -0.14868    0.415  0.304 -2.000
  14     O13  O -0.27202  0.24485 -0.08759    0.425  0.258 -2.000
  16     F15  F -0.11724  0.09175  0.24550    0.660 -0.958 -1.000
  15     F14  F  0.11723 -0.09175 -0.24550    0.660 -0.958 -1.000
  13     O12  O  0.27202 -0.24485  0.08759    0.425  0.258 -2.000
  11     O10  O  0.32471  0.35557  0.14868    0.415  0.304 -2.000
--------------------------------------------------------------------------------
   4     Fe3 Fe  0.00000  0.00000  0.00000          -10.662  3.000

Input a bond valence parameter: 3.000000
Bond valence of O11: -8.74286
Bond valence of O13: -8.92087
Bond valence of F15: -13.626
Bond valence of F14: -13.6261
Bond valence of O12: -8.92087
Bond valence of O10: -8.74286
Bond valence sum =62.580
Oxidation state of the cation: +3
Expected bond length = 3.256 Å

POLYHEDRON:
   4     Fe3 Fe  1.00000  0.00000  1.00000  ( 1, 0, 1)+ x, y, z
--------------------------------------------------------------------------------
  12     O11  O  0.67529 -0.35557  0.85132  ( 0,-1, 0)+ x, y, z
  14     O13  O  0.72798  0.24485  0.91241  ( 0, 0, 0)+ x, y, z
  16     F15  F  0.88276  0.09175  1.24550  ( 0, 0, 1)+ x, y, z
  15     F14  F  1.11723 -0.09175  0.75450  ( 1,-1, 0)+ x, y, z
  13     O12  O  1.27202 -0.24485  1.08759  ( 1,-1, 1)+ x, y, z
  11     O10  O  1.32471  0.35557  1.14868  ( 1, 0, 1)+ x, y, z
--------------------------------------------------------------------------------

l(Fe3-O11) =  2.19775(0) Å
l(Fe3-O13) =  2.19029(0) Å
l(Fe3-F15) =  2.03357(0) Å
l(Fe3-F14) =  2.03356(0) Å
l(Fe3-O12) =  2.19029(0) Å
l(Fe3-O10) =  2.19775(0) Å
---------------------------------------
Average bond length =  2.1405 Å
Polyhedral volume = 12.8898 Å^3
Distortion index (bond length) = 0.03332
```

Quadratic elongation = 1.0109
Bond angle variance = 29.9662 deg.^2
Effective coordination number = 5.6508

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
12	O11	O	0.67529	-0.35557	0.85132	0.415	0.304	-2.000
14	O13	O	0.72798	0.24485	0.91241	0.425	0.258	-2.000
16	F15	F	0.88276	0.09175	1.24550	0.660	-0.958	-1.000
15	F14	F	1.11723	-0.09175	0.75450	0.660	-0.958	-1.000
13	O12	O	1.27202	-0.24485	1.08759	0.425	0.258	-2.000
11	O10	O	1.32471	0.35557	1.14868	0.415	0.304	-2.000
4	Fe3	Fe	1.00000	0.00000	1.00000		-10.662	3.000

POLYHEDRON:

4	Fe3	Fe	0.00000	0.00000	1.00000	(0, 0, 1)+ x, y, z
12	O11	O	-0.32471	-0.35557	0.85132	(-1,-1, 0)+ x, y, z
14	O13	O	-0.27202	0.24485	0.91241	(-1, 0, 0)+ x, y, z
16	F15	F	-0.11724	0.09175	1.24550	(-1, 0, 1)+ x, y, z
15	F14	F	0.11723	-0.09175	0.75450	(0,-1, 0)+ x, y, z
13	O12	O	0.27202	-0.24485	1.08759	(0,-1, 1)+ x, y, z
11	O10	O	0.32471	0.35557	1.14868	(0, 0, 1)+ x, y, z

l(Fe3-O11) = 2.19775(0) Å
l(Fe3-O13) = 2.19029(0) Å
l(Fe3-F15) = 2.03357(0) Å
l(Fe3-F14) = 2.03356(0) Å
l(Fe3-O12) = 2.19029(0) Å
l(Fe3-O10) = 2.19775(0) Å

Average bond length = 2.1405 Å
Polyhedral volume = 12.8898 Å^3
Distortion index (bond length) = 0.03332
Quadratic elongation = 1.0109
Bond angle variance = 29.9662 deg.^2
Effective coordination number = 5.6508

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
12	O11	O	-0.32471	-0.35557	0.85132	0.415	0.304	-2.000
14	O13	O	-0.27202	0.24485	0.91241	0.425	0.258	-2.000
16	F15	F	-0.11724	0.09175	1.24550	0.660	-0.958	-1.000
15	F14	F	0.11723	-0.09175	0.75450	0.660	-0.958	-1.000
13	O12	O	0.27202	-0.24485	1.08759	0.425	0.258	-2.000
11	O10	O	0.32471	0.35557	1.14868	0.415	0.304	-2.000
4	Fe3	Fe	0.00000	0.00000	1.00000		-10.662	3.000

POLYHEDRON:

1	Li0	Li	0.26371	0.62117	0.78646	(0, 0, 0)+ x, y, z
10	O9	O	-0.10599	0.34912	0.66396	(-1, 0, 0)+ x, y, z
8	O7	O	0.40060	0.24710	0.59855	(0, 0, 0)+ x, y, z

```
  15     F14  F  0.11723  0.90825  0.75450  ( 0, 0, 0)+ x, y, z
  13     O12  O  0.27202  0.75515  1.08759  ( 0, 0, 1)+ x, y, z
  12     O11  O  0.67529  0.64443  0.85132  ( 0, 0, 0)+ x, y, z
--------------------------------------------------------------------------------

l(Li0-O9) =  2.07800(0) Å
l(Li0-O7) =  2.46425(0) Å
l(Li0-F14) =  1.91062(0) Å
l(Li0-O12) =  2.11578(0) Å
l(Li0-O11) =  2.04872(0) Å
---------------------------------------
Average bond length =  2.1235 Å
Polyhedral volume =  6.9062 Å^3
Distortion index (bond length) = 0.06419
Effective coordination number =  3.8579

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
  10      O9  O -0.10599  0.34912  0.66396   -0.213  0.306 -2.000
   8      O7  O  0.40060  0.24710  0.59855   -0.025  0.090 -2.000
  15     F14  F  0.11723  0.90825  0.75450   -0.342 -0.958 -1.000
  13     O12  O  0.27202  0.75515  1.08759   -0.186  0.258 -2.000
  12     O11  O  0.67529  0.64443  0.85132   -0.235  0.304 -2.000
--------------------------------------------------------------------------------
   1     Li0 Li  0.26371  0.62117  0.78646           4.575 -1.000

Input a bond valence parameter: -1.000000
Bond valence of O9: -0.000243861
Bond valence of O7: -8.58572e-05
Bond valence of F14: -0.000383359
Bond valence of O12: -0.000220188
Bond valence of O11: -0.000263943
Bond valence sum = 0.001
Oxidation state of the cation: -1
Expected bond length =-1.#IO Å

POLYHEDRON:
   3     Mn2 Mn  1.00000  1.00000  0.50000  ( 1, 1, 0)+ x, y, z
--------------------------------------------------------------------------------
   7      O6  O  0.59941  0.75290  0.40145  ( 0, 0, 0)+ x, y, z
  16     F15  F  0.88276  1.09175  0.24550  ( 0, 1, 0)+ x, y, z
  10      O9  O  0.89401  1.34912  0.66396  ( 0, 1, 0)+ x, y, z
   9      O8  O  1.10599  0.65088  0.33604  ( 1, 0, 0)+ x, y, z
  15     F14  F  1.11723  0.90825  0.75450  ( 1, 0, 0)+ x, y, z
   8      O7  O  1.40060  1.24710  0.59855  ( 1, 1, 0)+ x, y, z
--------------------------------------------------------------------------------

l(Mn2-O6) =  2.15521(0) Å
l(Mn2-F15) =  2.03824(0) Å
l(Mn2-O9) =  2.20535(0) Å
l(Mn2-O8) =  2.20535(0) Å
l(Mn2-F14) =  2.03824(0) Å
l(Mn2-O7) =  2.15521(0) Å
---------------------------------------
Average bond length =  2.1329 Å
Polyhedral volume = 12.8586 Å^3
Distortion index (bond length) = 0.02960
Quadratic elongation =  1.0052
Bond angle variance =  10.7819 deg.^2
Effective coordination number =  5.7154

Charge distribution
--------------------------------------------------------------------------------
```

```
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
   7      O6  O  0.59941  0.75290  0.40145    0.465  0.090 -2.000
  16     F15  F  0.88276  1.09175  0.24550    0.640 -0.958 -1.000
  10      O9  O  0.89401  1.34912  0.66396    0.394  0.306 -2.000
   9      O8  O  1.10599  0.65088  0.33604    0.394  0.306 -2.000
  15     F14  F  1.11723  0.90825  0.75450    0.640 -0.958 -1.000
   8      O7  O  1.40060  1.24710  0.59855    0.465  0.090 -2.000
--------------------------------------------------------------------------------
   3     Mn2 Mn  1.00000  1.00000  0.50000          -24.548  3.000

Input a bond valence parameter: 2.000000
Bond valence of O6: -0.657384
Bond valence of F15: -0.901808
Bond valence of O9: -0.574076
Bond valence of O8: -0.574076
Bond valence of F14: -0.90181
Bond valence of O7: -0.657377
Bond valence sum = 4.267
Oxidation state of the cation: +3
Expected bond length = 2.256 Å

POLYHEDRON:
   4     Fe3 Fe  1.00000  1.00000  0.00000  ( 1, 1, 0)+ x, y, z
--------------------------------------------------------------------------------
  12     O11  O  0.67529  0.64443 -0.14868  ( 0, 0,-1)+ x, y, z
  14     O13  O  0.72798  1.24485 -0.08759  ( 0, 1,-1)+ x, y, z
  16     F15  F  0.88276  1.09175  0.24550  ( 0, 1, 0)+ x, y, z
  15     F14  F  1.11723  0.90825 -0.24550  ( 1, 0,-1)+ x, y, z
  13     O12  O  1.27202  0.75515  0.08759  ( 1, 0, 0)+ x, y, z
  11     O10  O  1.32471  1.35557  0.14868  ( 1, 1, 0)+ x, y, z
--------------------------------------------------------------------------------

l(Fe3-O11) =  2.19775(0) Å
l(Fe3-O13) =  2.19029(0) Å
l(Fe3-F15) =  2.03357(0) Å
l(Fe3-F14) =  2.03356(0) Å
l(Fe3-O12) =  2.19029(0) Å
l(Fe3-O10) =  2.19775(0) Å
--------------------------------------
Average bond length =  2.1405 Å
Polyhedral volume = 12.8898 Å^3
Distortion index (bond length) = 0.03332
Quadratic elongation =  1.0109
Bond angle variance =  29.9663 deg.^2
Effective coordination number =  5.6508

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
  12     O11  O  0.67529  0.64443 -0.14868    0.415  0.304 -2.000
  14     O13  O  0.72798  1.24485 -0.08759    0.425  0.258 -2.000
  16     F15  F  0.88276  1.09175  0.24550    0.660 -0.958 -1.000
  15     F14  F  1.11723  0.90825 -0.24550    0.660 -0.958 -1.000
  13     O12  O  1.27202  0.75515  0.08759    0.425  0.258 -2.000
  11     O10  O  1.32471  1.35557  0.14868    0.415  0.304 -2.000
--------------------------------------------------------------------------------
   4     Fe3 Fe  1.00000  1.00000  0.00000          -10.662  3.000

Input a bond valence parameter: 2.000000
Bond valence of O11: -0.585982
```

```
Bond valence of O13: -0.597914
Bond valence of F15: -0.913271
Bond valence of F14: -0.913279
Bond valence of O12: -0.597914
Bond valence of O10: -0.585982
Bond valence sum = 4.194
Oxidation state of the cation: +3
Expected bond length = 2.256 Å

POLYHEDRON:
   4     Fe3 Fe  1.00000  0.00000  1.00000  ( 1, 0, 1)+ x, y, z
--------------------------------------------------------------------------------
  12     O11  O  0.67529 -0.35557  0.85132  ( 0,-1, 0)+ x, y, z
  14     O13  O  0.72798  0.24485  0.91241  ( 0, 0, 0)+ x, y, z
  16     F15  F  0.88276  0.09175  1.24550  ( 0, 0, 1)+ x, y, z
  15     F14  F  1.11723 -0.09175  0.75450  ( 1,-1, 0)+ x, y, z
  13     O12  O  1.27202 -0.24485  1.08759  ( 1,-1, 1)+ x, y, z
  11     O10  O  1.32471  0.35557  1.14868  ( 1, 0, 1)+ x, y, z
--------------------------------------------------------------------------------

l(Fe3-O11) =  2.19775(0) Å
l(Fe3-O13) =  2.19029(0) Å
l(Fe3-F15) =  2.03357(0) Å
l(Fe3-F14) =  2.03356(0) Å
l(Fe3-O12) =  2.19029(0) Å
l(Fe3-O10) =  2.19775(0) Å
---------------------------------------
Average bond length =  2.1405 Å
Polyhedral volume = 12.8898 Å^3
Distortion index (bond length) = 0.03332
Quadratic elongation =  1.0109
Bond angle variance =  29.9662 deg.^2
Effective coordination number =  5.6508

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
  12     O11  O  0.67529 -0.35557  0.85132    0.415  0.304 -2.000
  14     O13  O  0.72798  0.24485  0.91241    0.425  0.258 -2.000
  16     F15  F  0.88276  0.09175  1.24550    0.660 -0.958 -1.000
  15     F14  F  1.11723 -0.09175  0.75450    0.660 -0.958 -1.000
  13     O12  O  1.27202 -0.24485  1.08759    0.425  0.258 -2.000
  11     O10  O  1.32471  0.35557  1.14868    0.415  0.304 -2.000
--------------------------------------------------------------------------------
   4     Fe3 Fe  1.00000  0.00000  1.00000          -10.662  3.000

Input a bond valence parameter: 2.000000
Bond valence of O11: -0.585982
Bond valence of O13: -0.597914
Bond valence of F15: -0.913271
Bond valence of F14: -0.913279
Bond valence of O12: -0.597914
Bond valence of O10: -0.585982
Bond valence sum = 4.194
Oxidation state of the cation: +3
Expected bond length = 2.256 Å

POLYHEDRON:
   6      S5  S  0.67494  0.36767  0.75545  ( 0, 0, 0)+ x, y, z
--------------------------------------------------------------------------------
   8      O7  O  0.40060  0.24710  0.59855  ( 0, 0, 0)+ x, y, z
  14     O13  O  0.72798  0.24485  0.91241  ( 0, 0, 0)+ x, y, z
  10      O9  O  0.89401  0.34912  0.66396  ( 0, 0, 0)+ x, y, z
  12     O11  O  0.67529  0.64443  0.85132  ( 0, 0, 0)+ x, y, z
```

```
--------------------------------------------------------------------------------

l(S5-O7) =  1.47708(0) Å
l(S5-O13) =  1.49282(0) Å
l(S5-O9) =  1.49815(0) Å
l(S5-O11) =  1.49983(0) Å
---------------------------------------
Average bond length =  1.4920 Å
Polyhedral volume =  1.7023 Å^3
Distortion index (bond length) = 0.00499
Quadratic elongation =  1.0009
Bond angle variance =   3.1992 deg.^2
Effective coordination number =  3.9949

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
   8      O7  O  0.40060  0.24710  0.59855   -0.530  0.090 -2.000
  14     O13  O  0.72798  0.24485  0.91241   -0.498  0.258 -2.000
  10      O9  O  0.89401  0.34912  0.66396   -0.488  0.306 -2.000
  12     O11  O  0.67529  0.64443  0.85132   -0.484  0.304 -2.000
--------------------------------------------------------------------------------
   6      S5  S  0.67494  0.36767  0.75545          22.029 -2.000

Input a bond valence parameter: -2.000000
Bond valence of O7: -8.29299e-05
Bond valence of O13: -7.94752e-05
Bond valence of O9: -7.83388e-05
Bond valence of O11: -7.79849e-05
Bond valence sum = 0.000
Oxidation state of the cation: -2
Expected bond length =-1.#IO Å

POLYHEDRON:
   5      S4  S  0.32506  0.63233  0.24455  ( 0, 0, 0)+ x, y, z
--------------------------------------------------------------------------------
  11     O10  O  0.32471  0.35557  0.14868  ( 0, 0, 0)+ x, y, z
   9      O8  O  0.10599  0.65088  0.33604  ( 0, 0, 0)+ x, y, z
  13     O12  O  0.27202  0.75515  0.08759  ( 0, 0, 0)+ x, y, z
   7      O6  O  0.59941  0.75290  0.40145  ( 0, 0, 0)+ x, y, z
--------------------------------------------------------------------------------

l(S4-O10) =  1.49983(0) Å
l(S4-O8) =  1.49815(0) Å
l(S4-O12) =  1.49282(0) Å
l(S4-O6) =  1.47708(0) Å
---------------------------------------
Average bond length =  1.4920 Å
Polyhedral volume =  1.7023 Å^3
Distortion index (bond length) = 0.00499
Quadratic elongation =  1.0009
Bond angle variance =   3.1994 deg.^2
Effective coordination number =  3.9949

Charge distribution
--------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
--------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
  11     O10  O  0.32471  0.35557  0.14868   -0.484  0.304 -2.000
   9      O8  O  0.10599  0.65088  0.33604   -0.488  0.306 -2.000
  13     O12  O  0.27202  0.75515  0.08759   -0.498  0.258 -2.000
```

```
   7      O6  O  0.59941  0.75290  0.40145   -0.530  0.090 -2.000
-------------------------------------------------------------------------------
   5      S4  S  0.32506  0.63233  0.24455          22.031 -2.000


POLYHEDRON:
   5      S4  S  0.32506  0.63233  0.24455  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------
  11     O10  O  0.32471  0.35557  0.14868  ( 0, 0, 0)+ x, y, z
   9      O8  O  0.10599  0.65088  0.33604  ( 0, 0, 0)+ x, y, z
  13     O12  O  0.27202  0.75515  0.08759  ( 0, 0, 0)+ x, y, z
   7      O6  O  0.59941  0.75290  0.40145  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------

l(S4-O10) =  1.49983(0) Å
l(S4-O8) =  1.49815(0) Å
l(S4-O12) =  1.49282(0) Å
l(S4-O6) =  1.47708(0) Å
---------------------------------------
Average bond length =  1.4920 Å
Polyhedral volume =  1.7023 Å^3
Distortion index (bond length) = 0.00499
Quadratic elongation =  1.0009
Bond angle variance =   3.1994 deg.^2
Effective coordination number =  3.9949

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
  11     O10  O  0.32471  0.35557  0.14868   -0.484  0.304 -2.000
   9      O8  O  0.10599  0.65088  0.33604   -0.488  0.306 -2.000
  13     O12  O  0.27202  0.75515  0.08759   -0.498  0.258 -2.000
   7      O6  O  0.59941  0.75290  0.40145   -0.530  0.090 -2.000
-------------------------------------------------------------------------------
   5      S4  S  0.32506  0.63233  0.24455          22.031 -2.000

Input a bond valence parameter: -2.000000
Bond valence of O10: -7.79852e-05
Bond valence of O8: -7.83388e-05
Bond valence of O12: -7.94752e-05
Bond valence of O6: -8.29291e-05
Bond valence sum = 0.000
Oxidation state of the cation: -2
Expected bond length =-1.#IO Å

C:\simulation\DFT Li-ion battery simulation\Tevorite and triplets\LiFeNSF_triclinic
P-12.cif
================================================================================
=
Title               LiFeNSF

Lattice type        P
Space group name    P 1
Space group number  1
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 5.25236  5.59647  7.40296 107.2483 107.2924  97.0660

Unit-cell volume = 193.034809 Å^3

Structure parameters
```

			x	y	z	Occ.	B	Site Sym.
1	Li	Li0	0.26371	0.62117	0.78646	1.000	1.000	1a 1
2	Li	Li1	0.73628	0.37883	0.21354	1.000	1.000	1a 1
3	Ni	Ni2	0.00000	0.00000	0.50000	1.000	1.000	1a 1
4	Fe	Fe3	0.00000	0.00000	0.00000	1.000	1.000	1a 1
5	S	S4	0.32506	0.63233	0.24455	1.000	1.000	1a 1
6	S	S5	0.67494	0.36767	0.75545	1.000	1.000	1a 1
7	O	O6	0.59941	0.75290	0.40145	1.000	1.000	1a 1
8	O	O7	0.40060	0.24710	0.59855	1.000	1.000	1a 1
9	O	O8	0.10599	0.65088	0.33604	1.000	1.000	1a 1
10	O	O9	0.89401	0.34912	0.66396	1.000	1.000	1a 1
11	O	O10	0.32471	0.35557	0.14868	1.000	1.000	1a 1
12	O	O11	0.67529	0.64443	0.85132	1.000	1.000	1a 1
13	O	O12	0.27202	0.75515	0.08759	1.000	1.000	1a 1
14	O	O13	0.72798	0.24485	0.91241	1.000	1.000	1a 1
15	F	F14	0.11723	0.90825	0.75450	1.000	1.000	1a 1
16	F	F15	0.88276	0.09175	0.24550	1.000	1.000	1a 1

==========

Number of polygons and unique vertices on isosurface = 0 (0)
80 atoms, 90 bonds, 16 polyhedra; CPU time = 5 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 10 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 4 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

```
================================================================================
=
Title               li2 fe2 s2 o8 f2

Lattice type        P
Space group name    P 1
Space group number  1
Setting number      1

Lattice parameters

   a        b        c       alpha    beta     gamma
 5.25236  5.59647  7.40296 107.2483 107.2924  97.0660

Unit-cell volume = 193.034809 Å^3

Structure parameters

                       x          y          z          Occ.     B    Site
Sym.
   1 Li  Li0          0.26371    0.62117    0.78646    1.000    1.000    1a
1
   2 Li  Li1          0.73628    0.37883    0.21354    1.000    1.000    1a
1
   3 Ni  Ni2          0.00000    0.00000    0.50000    1.000    1.000    1a
1
   4 Fe  Fe3          0.00000    0.00000    0.00000    1.000    1.000    1a
1
   5 S   S4           0.32506    0.63233    0.24455    1.000    1.000    1a
1
   6 S   S5           0.67494    0.36767    0.75545    1.000    1.000    1a
1
   7 O   O6           0.59941    0.75290    0.40145    1.000    1.000    1a
1
   8 O   O7           0.40060    0.24710    0.59855    1.000    1.000    1a
1
   9 O   O8           0.10599    0.65088    0.33604    1.000    1.000    1a
1
  10 O   O9           0.89401    0.34912    0.66396    1.000    1.000    1a
1
  11 O   O10          0.32471    0.35557    0.14868    1.000    1.000    1a
1
  12 O   O11          0.67529    0.64443    0.85132    1.000    1.000    1a
1
  13 O   O12          0.27202    0.75515    0.08759    1.000    1.000    1a
1
  14 O   O13          0.72798    0.24485    0.91241    1.000    1.000    1a
1
  15 F   F14          0.11723    0.90825    0.75450    1.000    1.000    1a
1
  16 F   F15          0.88276    0.09175    0.24550    1.000    1.000    1a
1
================================================================================
=
```

Number of polygons and unique vertices on isosurface = 0 (0)
80 atoms, 90 bonds, 16 polyhedra; CPU time = 3 ms

POLYHEDRON:

3	Ni2	Ni	1.00000	1.00000	0.50000	(1, 1, 0)+ x, y, z
7	O6	O	0.59941	0.75290	0.40145	(0, 0, 0)+ x, y, z
16	F15	F	0.88276	1.09175	0.24550	(0, 1, 0)+ x, y, z
10	O9	O	0.89401	1.34912	0.66396	(0, 1, 0)+ x, y, z
9	O8	O	1.10599	0.65088	0.33604	(1, 0, 0)+ x, y, z
15	F14	F	1.11723	0.90825	0.75450	(1, 0, 0)+ x, y, z
8	O7	O	1.40060	1.24710	0.59855	(1, 1, 0)+ x, y, z

l(Ni2-O6) = 2.15521(0) Å
l(Ni2-F15) = 2.03824(0) Å
l(Ni2-O9) = 2.20535(0) Å
l(Ni2-O8) = 2.20535(0) Å
l(Ni2-F14) = 2.03824(0) Å
l(Ni2-O7) = 2.15521(0) Å

Average bond length = 2.1329 Å
Polyhedral volume = 12.8586 Å^3
Distortion index (bond length) = 0.02960
Quadratic elongation = 1.0052
Bond angle variance = 10.7819 deg.^2
Effective coordination number = 5.7154

Charge distribution

delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)

			x	y	z	delta_q	Q	q
7	O6	O	0.59941	0.75290	0.40145	0.310	0.245	-2.000
16	F15	F	0.88276	1.09175	0.24550	0.427	-0.525	-1.000
10	O9	O	0.89401	1.34912	0.66396	0.298	0.437	-2.000
9	O8	O	1.10599	0.65088	0.33604	0.263	0.437	-2.000
15	F14	F	1.11723	0.90825	0.75450	0.327	-0.525	-1.000
8	O7	O	1.40060	1.24710	0.59855	0.310	0.245	-2.000
3	Ni2	Ni	1.00000	1.00000	0.50000		-5.845	2.000

Input a bond valence parameter: 2.000000
Bond valence of O6: -0.657384
Bond valence of F15: -0.901808
Bond valence of O9: -0.574076
Bond valence of O8: -0.574076
Bond valence of F14: -0.90181
Bond valence of O7: -0.657377
Bond valence sum = 4.267
Oxidation state of the cation: +2
Expected bond length = 2.406 Å

POLYHEDRON:

4	Fe3	Fe	1.00000	0.00000	1.00000	(1, 0, 1)+ x, y, z
12	O11	O	0.67529	-0.35557	0.85132	(0,-1, 0)+ x, y, z
14	O13	O	0.72798	0.24485	0.91241	(0, 0, 0)+ x, y, z
16	F15	F	0.88276	0.09175	1.24550	(0, 0, 1)+ x, y, z
15	F14	F	1.11723	-0.09175	0.75450	(1,-1, 0)+ x, y, z
13	O12	O	1.27202	-0.24485	1.08759	(1,-1, 1)+ x, y, z
11	O10	O	1.32471	0.35557	1.14868	(1, 0, 1)+ x, y, z

l(Fe3-O11) = 2.19775(0) Å

```
l(Fe3-O13) =  2.19029(0) Å
l(Fe3-F15) =  2.03357(0) Å
l(Fe3-F14) =  2.03356(0) Å
l(Fe3-O12) =  2.19029(0) Å
l(Fe3-O10) =  2.19775(0) Å
---------------------------------------
Average bond length =  2.1405 Å
Polyhedral volume = 12.8898 Å^3
Distortion index (bond length) = 0.03332
Quadratic elongation =  1.0109
Bond angle variance =  29.9662 deg.^2
Effective coordination number =  5.6508

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
  12     O11  O  0.67529 -0.35557  0.85132    0.277  0.442 -2.000
  14     O13  O  0.72798  0.24485  0.91241    0.284  0.400 -2.000
  16     F15  F  0.88276  0.09175  1.24550    0.440 -0.525 -1.000
  15     F14  F  1.11723 -0.09175  0.75450    0.440 -0.525 -1.000
  13     O12  O  1.27202 -0.24485  1.08759    0.284  0.400 -2.000
  11     O10  O  1.32471  0.35557  1.14868    0.277  0.442 -2.000
-------------------------------------------------------------------------------
   4     Fe3 Fe  1.00000  0.00000  1.00000          -3.658  2.000

Input a bond valence parameter: 2.000000
Bond valence of O11: -0.585982
Bond valence of O13: -0.597914
Bond valence of F15: -0.913271
Bond valence of F14: -0.913279
Bond valence of O12: -0.597914
Bond valence of O10: -0.585982
Bond valence sum = 4.194
Oxidation state of the cation: +2
Expected bond length = 2.406 Å

POLYHEDRON:
   1     Li0 Li  0.26371  0.62117  0.78646  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------
  10      O9  O -0.10599  0.34912  0.66396  (-1, 0, 0)+ x, y, z
   8      O7  O  0.40060  0.24710  0.59855  ( 0, 0, 0)+ x, y, z
  15     F14  F  0.11723  0.90825  0.75450  ( 0, 0, 0)+ x, y, z
  13     O12  O  0.27202  0.75515  1.08759  ( 0, 0, 1)+ x, y, z
  12     O11  O  0.67529  0.64443  0.85132  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------

l(Li0-O9) =  2.07800(0) Å
l(Li0-O7) =  2.46425(0) Å
l(Li0-F14) =  1.91062(0) Å
l(Li0-O12) =  2.11578(0) Å
l(Li0-O11) =  2.04872(0) Å
---------------------------------------
Average bond length =  2.1235 Å
Polyhedral volume =  6.9062 Å^3
Distortion index (bond length) = 0.06419
Effective coordination number =  3.8579

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                   x        y        z      delta_q    Q      q
```

```
  10      O9  O -0.10599  0.34912  0.66396   -0.213  0.437 -2.000
   8      O7  O  0.40060  0.24710  0.59855   -0.025  0.245 -2.000
  15     F14  F  0.11723  0.90825  0.75450   -0.342 -0.525 -1.000
  13     O12  O  0.27202  0.75515  1.08759   -0.186  0.400 -2.000
  12     O11  O  0.67529  0.64443  0.85132   -0.235  0.442 -2.000
-------------------------------------------------------------------------------
   1     Li0 Li  0.26371  0.62117  0.78646           2.516 -1.000

Input a bond valence parameter: -1.000000
Bond valence of O9: -0.000243861
Bond valence of O7: -8.58572e-05
Bond valence of F14: -0.000383359
Bond valence of O12: -0.000220188
Bond valence of O11: -0.000263943
Bond valence sum = 0.001
Oxidation state of the cation: -1
Expected bond length =-1.#IO Å

POLYHEDRON:
   6      S5  S  0.67494  0.36767  0.75545  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------
   8      O7  O  0.40060  0.24710  0.59855  ( 0, 0, 0)+ x, y, z
  14     O13  O  0.72798  0.24485  0.91241  ( 0, 0, 0)+ x, y, z
  10      O9  O  0.89401  0.34912  0.66396  ( 0, 0, 0)+ x, y, z
  12     O11  O  0.67529  0.64443  0.85132  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------

l(S5-O7) =  1.47708(0) Å
l(S5-O13) =  1.49282(0) Å
l(S5-O9) =  1.49815(0) Å
l(S5-O11) =  1.49983(0) Å
---------------------------------------
Average bond length =  1.4920 Å
Polyhedral volume =  1.7023 Å^3
Distortion index (bond length) = 0.00499
Quadratic elongation =  1.0009
Bond angle variance =   3.1992 deg.^2
Effective coordination number =  3.9949

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
   8      O7  O  0.40060  0.24710  0.59855   -0.530  0.245 -2.000
  14     O13  O  0.72798  0.24485  0.91241   -0.498  0.400 -2.000
  10      O9  O  0.89401  0.34912  0.66396   -0.488  0.437 -2.000
  12     O11  O  0.67529  0.64443  0.85132   -0.484  0.442 -2.000
-------------------------------------------------------------------------------
   6      S5  S  0.67494  0.36767  0.75545          11.236 -2.000

Input a bond valence parameter: -2.000000
Bond valence of O7: -8.29299e-05
Bond valence of O13: -7.94752e-05
Bond valence of O9: -7.83388e-05
Bond valence of O11: -7.79849e-05
Bond valence sum = 0.000
Oxidation state of the cation: -2
Expected bond length =-1.#IO Å

POLYHEDRON:
   2     Li1 Li  0.73628  0.37883  0.21354  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------
  11     O10  O  0.32471  0.35557  0.14868  ( 0, 0, 0)+ x, y, z
  14     O13  O  0.72798  0.24485 -0.08759  ( 0, 0,-1)+ x, y, z
  16     F15  F  0.88276  0.09175  0.24550  ( 0, 0, 0)+ x, y, z
```

```
   7      O6  O  0.59941  0.75290  0.40145  ( 0, 0, 0)+ x, y, z
   9      O8  O  1.10599  0.65088  0.33604  ( 1, 0, 0)+ x, y, z
-------------------------------------------------------------------------------

l(Li1-O10) =  2.04872(0) Å
l(Li1-O13) =  2.11578(0) Å
l(Li1-F15) =  1.91062(0) Å
l(Li1-O6) =  2.46424(0) Å
l(Li1-O8) =  2.07800(0) Å
---------------------------------------
Average bond length =  2.1235 Å
Polyhedral volume =  6.9062 Å^3
Distortion index (bond length) = 0.06419
Effective coordination number =  3.8579

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
  11     O10  O  0.32471  0.35557  0.14868   -0.235  0.442 -2.000
  14     O13  O  0.72798  0.24485 -0.08759   -0.186  0.400 -2.000
  16     F15  F  0.88276  0.09175  0.24550   -0.342 -0.525 -1.000
   7      O6  O  0.59941  0.75290  0.40145   -0.025  0.245 -2.000
   9      O8  O  1.10599  0.65088  0.33604   -0.213  0.437 -2.000
-------------------------------------------------------------------------------
   2     Li1 Li  0.73628  0.37883  0.21354           2.516 -1.000

Input a bond valence parameter: -1.000000
Bond valence of O10: -0.000263943
Bond valence of O13: -0.000220188
Bond valence of F15: -0.000383362
Bond valence of O6: -8.58579e-05
Bond valence of O8: -0.000243861
Bond valence sum = 0.001
Oxidation state of the cation: -1
Expected bond length =-1.#IO Å

POLYHEDRON:
   5      S4  S  0.32506  0.63233  0.24455  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------
  11     O10  O  0.32471  0.35557  0.14868  ( 0, 0, 0)+ x, y, z
   9      O8  O  0.10599  0.65088  0.33604  ( 0, 0, 0)+ x, y, z
  13     O12  O  0.27202  0.75515  0.08759  ( 0, 0, 0)+ x, y, z
   7      O6  O  0.59941  0.75290  0.40145  ( 0, 0, 0)+ x, y, z
-------------------------------------------------------------------------------

l(S4-O10) =  1.49983(0) Å
l(S4-O8) =  1.49815(0) Å
l(S4-O12) =  1.49282(0) Å
l(S4-O6) =  1.47708(0) Å
---------------------------------------
Average bond length =  1.4920 Å
Polyhedral volume =  1.7023 Å^3
Distortion index (bond length) = 0.00499
Quadratic elongation =  1.0009
Bond angle variance =   3.1994 deg.^2
Effective coordination number =  3.9949

Charge distribution
-------------------------------------------------------------------------------
delta_q: Fraction of the charge received by the ion
Q: Total charge received by the ion
q: Formal charge (oxidation number)
-------------------------------------------------------------------------------
                  x        y        z      delta_q    Q      q
```

```
  11     O10  O  0.32471  0.35557  0.14868   -0.484  0.442 -2.000
   9      O8  O  0.10599  0.65088  0.33604   -0.488  0.437 -2.000
  13     O12  O  0.27202  0.75515  0.08759   -0.498  0.400 -2.000
   7      O6  O  0.59941  0.75290  0.40145   -0.530  0.245 -2.000
-------------------------------------------------------------------------------
   5      S4  S  0.32506  0.63233  0.24455          11.236 -2.000

Input a bond valence parameter: -2.000000
Bond valence of O10: -7.79852e-05
Bond valence of O8: -7.83388e-05
Bond valence of O12: -7.94752e-05
Bond valence of O6: -8.29291e-05
Bond valence sum = 0.000
Oxidation state of the cation: -2
Expected bond length =-1.#IO Å
```