Suppoting Informations

Exploring the influence of hydrogen bond donors within deep eutectic solvents on the extraction of metals during the recycling process of lithium-ion batteries

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Table S1. Detailed synthetic temperature and time for the DESs.

DES	Synthesis Temperature (°C)	Synthesis Time (min)
EG:ChCl	80	10
Gly:ChCl	80	10
Urea:ChCl	90	20
TUrea:ChCl	110	30
Ox Acid:ChCl	100	30
Benz Acid:ChCl	110	30

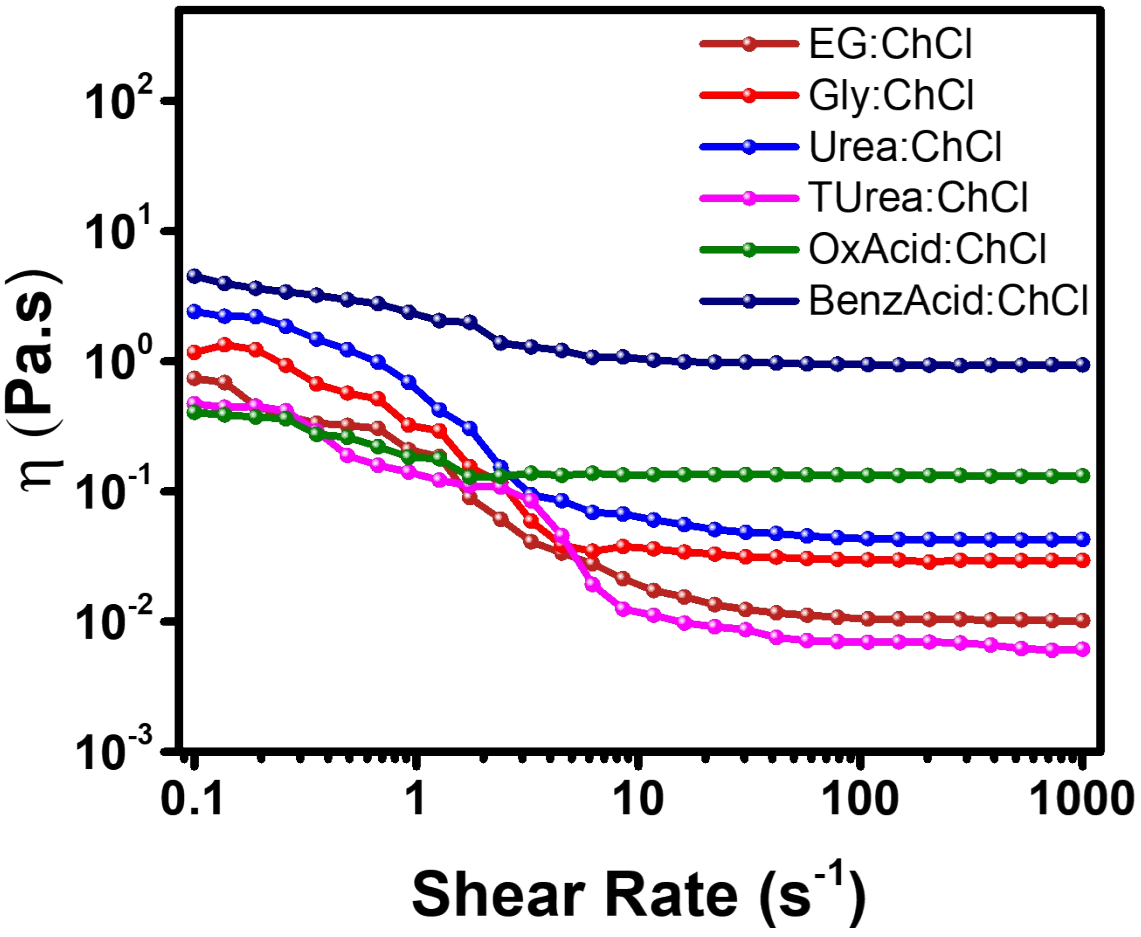

Figure S1. Viscosity vs shear rate curves of the DESs.

Temperature dependent viscosities and activation energy calculation:

The viscosities of all NADES decreased with increasing temperature, which can be correlated with the Arrhenius model according to the following equation,

$$\eta = \eta_0 e^{(E_a/RT)} \quad \text{(Eq. S1)}$$

Where,

η = viscosity (Pa.s)

η_0 = pre-exponential factor (Pa.s)

E_a = activation energy ($Jmol^{-1}$)

R = ideal gas constant ($Jmol^{-1}K^{-1}$)

T = temperature (K)

The logarithmic form of Equation S1 for the prepared NADES is plotted in Figure S6b. Note that the slopes of the plots indicate E_a, representing the activation energy barriers of NADES to shear stress.

Table S2. E_a values as a function of temperature

DES	E_a ($Jmol^{-1}$)	R^2
EG:ChCl	250.4041	0.99291
Gly:ChCl	384.5321	0.93013
Urea:ChCl	517.3202	0.98328
TUrea:ChCl	343.6372	0.95644
Ox Acid:ChCl	538.1285	0.98734
Benz Acid:ChCl	1493.625	0.97605

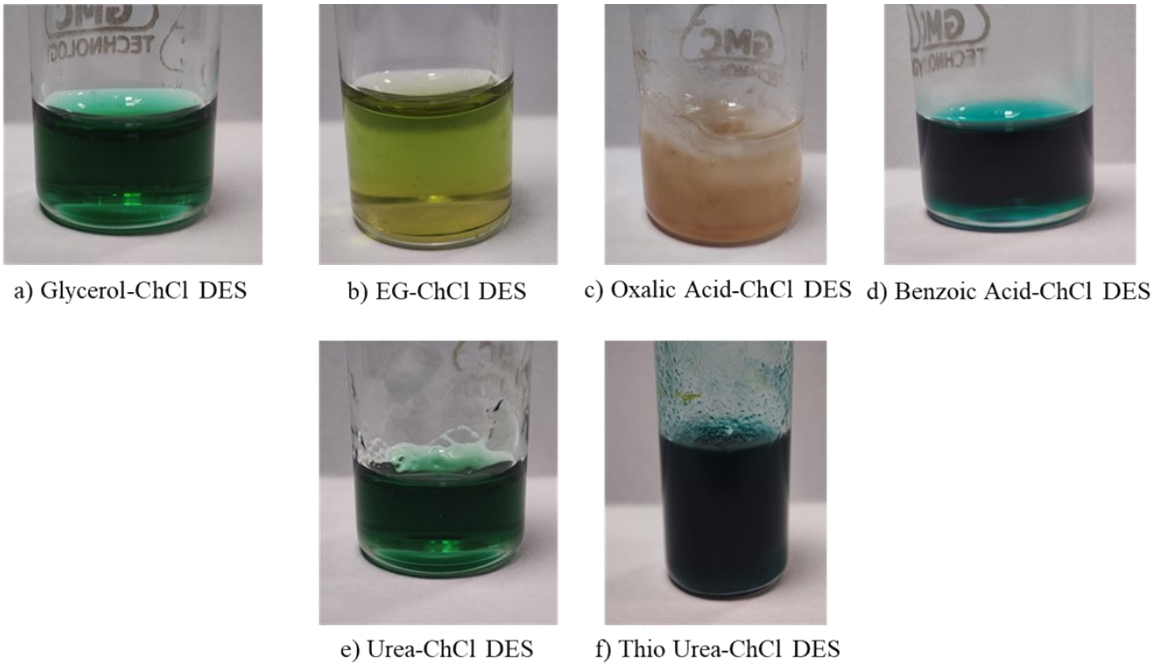

Figure S2. Images of DESs after the leaching and filtration process of LIB powder for **a.** Gly-ChCl, **b.** EG-ChCl, **c.** Ox Acid-ChCl, **d.** Benz Acid-ChCl, **e.** Urea-ChCl and **f.** Thiourea-ChCl DESs.

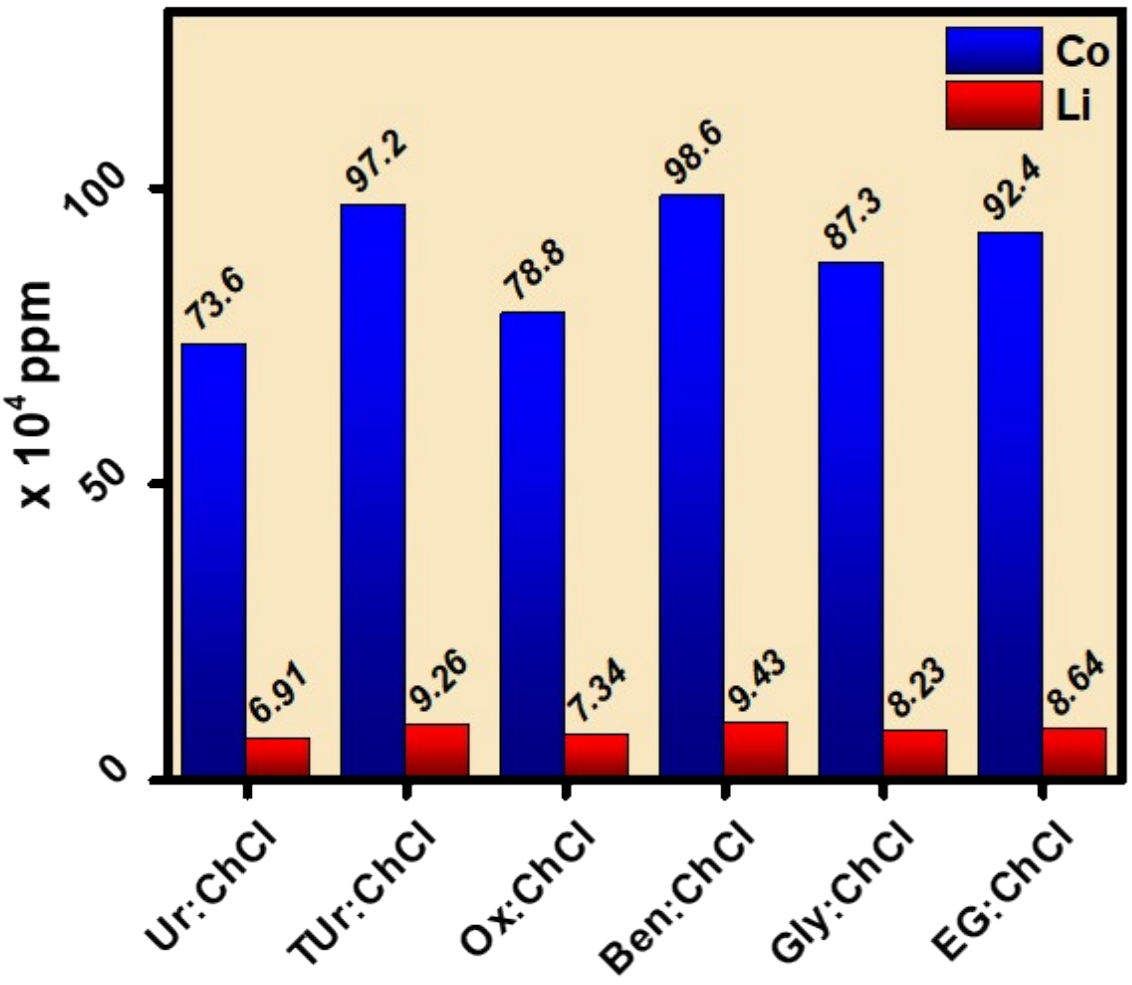

Figure S3. Effective amount of leached metal Cobalt and Lithium form the LCO powder by different DESs.

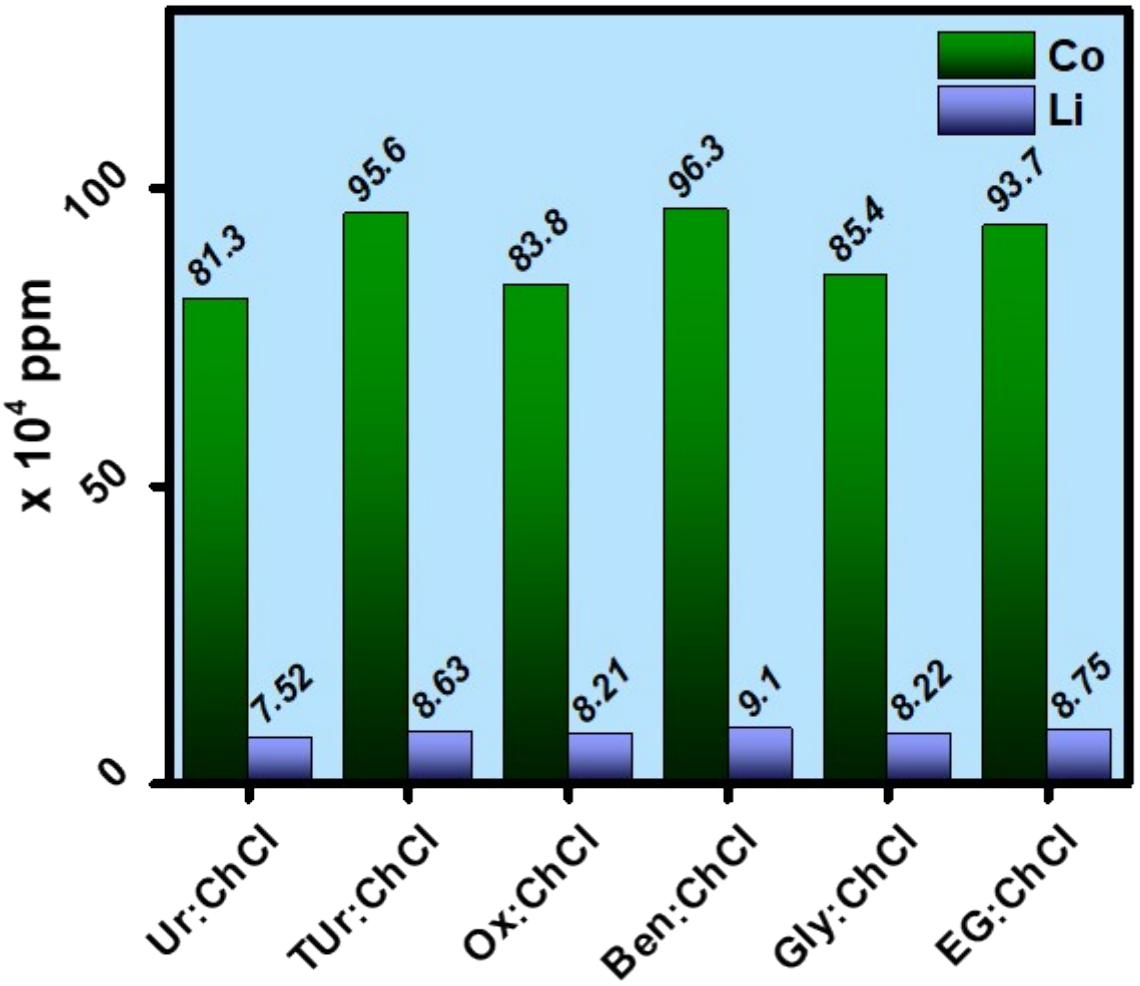

Figure S4. Effective amount of leached metal Cobalt and Lithium form the LIB powder by different DESs.

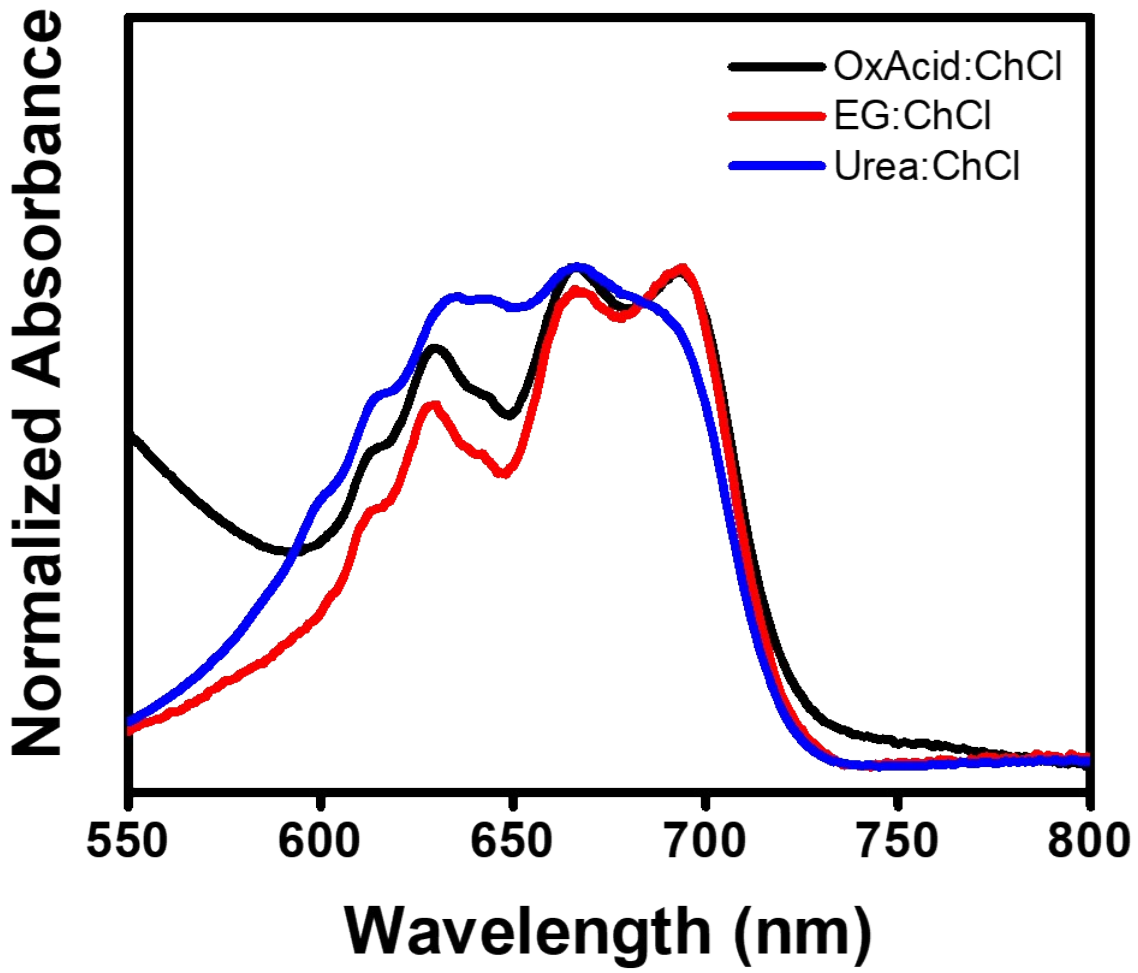

Figure S5. UV-visible spectra of the EG:ChCl, Urea:ChCl and OxAcid:ChCl DES after LCO leaching showing the peaks of Co(II)-coordinated complexations in the range of 600-700 nm.

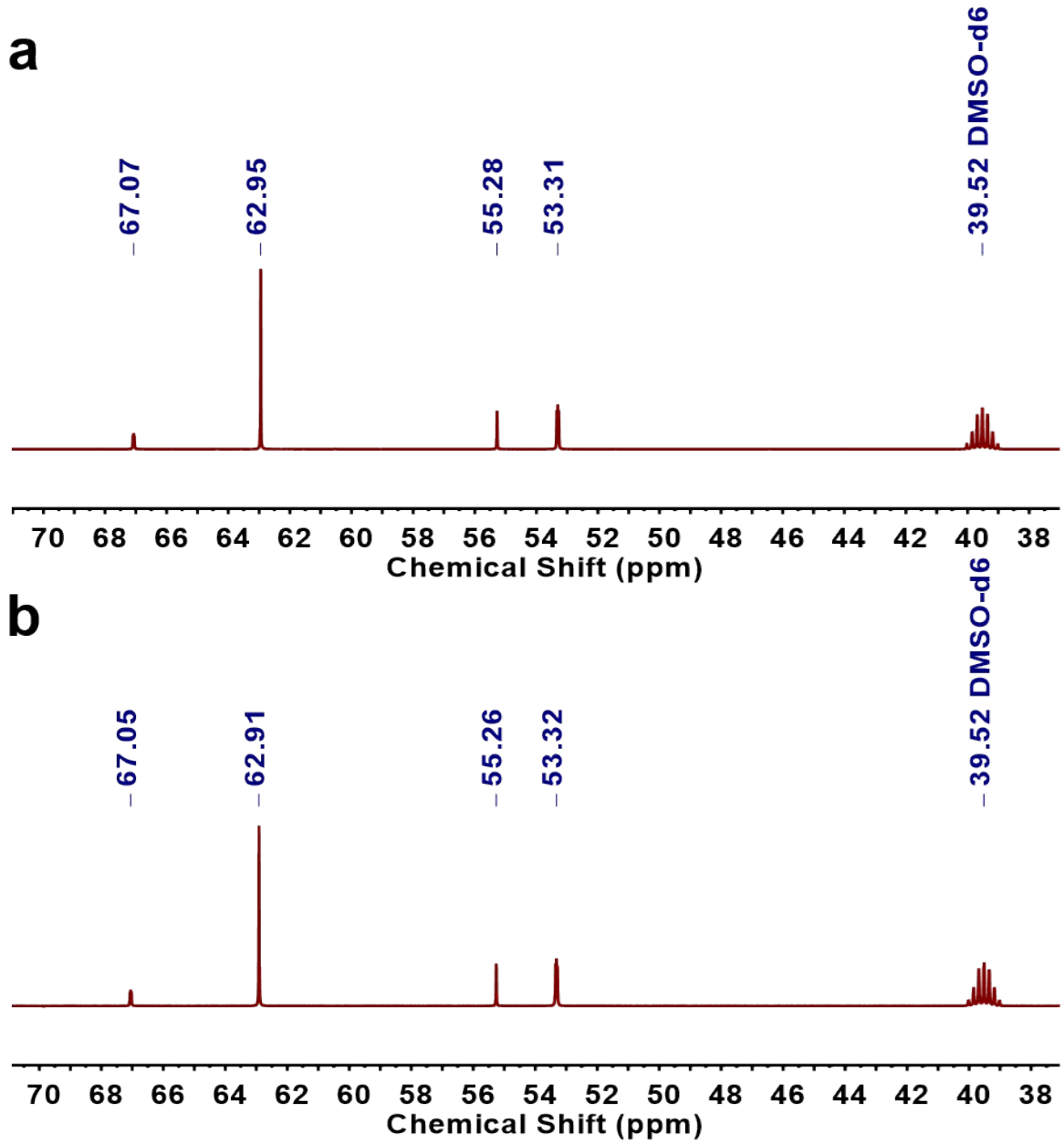

Figure S6. ^{13}C-NMR spectra of the EG:ChCl DES **a.** before leaching and **b.** after leaching.

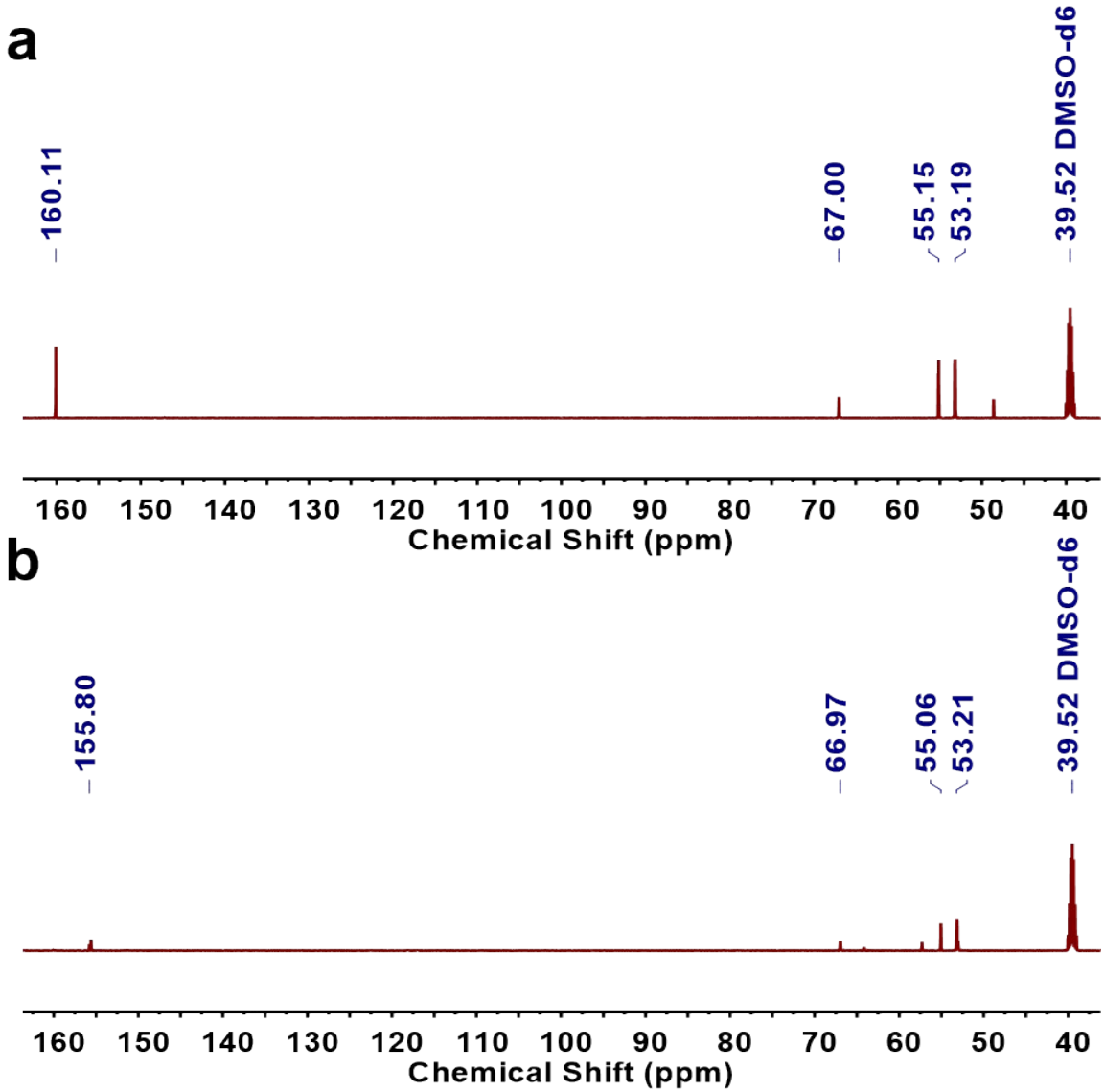

Figure S7. ^{13}C-NMR spectra of the Urea:ChCl DES **a.** before leaching and **b.** after leaching.

Table S3. The estimated yields of the recovered Co_3O_4 from LCO powder with the various HBD-functionalized DESs.

DES	LCO taken (mg)	Co_3O_4 recovered (mg)
EG:ChCl	30	9.11
OxAcid:ChCl	30	11.3
Urea:ChCl	30	13.4

Table S4. The estimated cost for the components used to produce DESs and Acid based solvents used for LIB leaching processes.

NAME OF DES COMPONENT	PRICE IN USD	COST OF ACID BASED ALTERNATIVE	PRICE IN USD
Choline Chloride	3.13 $ per Kg	Hydrochloric Acid	3.15 $ per Litre
Ethylene Glycol	1.08 $ per Litre	Nitric Acid	1.14 $ per Litre
Glycerol	0.78 $ per Kg	Sulphuric Acid	0.54 $ per Kg
Benzoic Acid	1.02 $ per Kg	Ascorbic Acid	3.61 $ per Kg
Oxalic Acid	0.54 $ per Kg		
Thio Urea	3.01 $ per Kg		
Urea	0.72 $ per Kg		