Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Investigation of glycerol hydrogen-bonding networks in choline chloride/glycerol eutectic-forming liquids using neutron diffraction

Adam H. Turner*,†,‡ and John D. Holbrey*,†

† *The QUILL Research Centre, School of Chemistry and Chemical Engineering, The Queen's University of Belfast, Belfast BT9 5AG, UK*

‡ *Department of Chemistry, Ateneo de Manila University, Quezon City 1108, Philippines*

E-mail: aturner@ateneo.edu; j.holbrey@qub.ac.uk

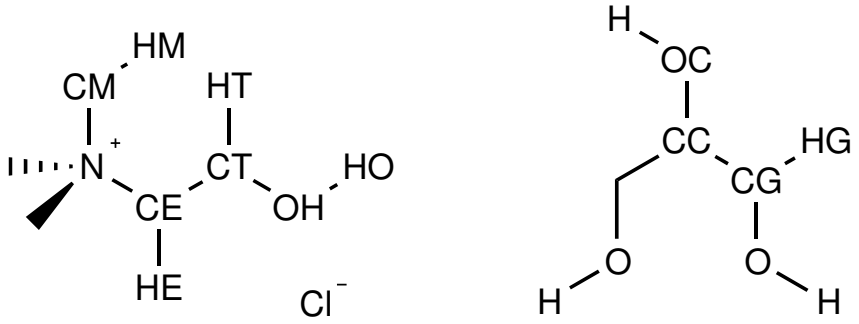

Figure S1: Atom types assigned to the choline chloride and glycerol components used in the EPSR simulation of the neutron scattering data.

Table S1: Initial Lennard-Jones (ε and σ) and charge (q) parameters used for the reference potential of the Empirical Potential Structure Refinement model for both systems derived from the literature, and OPLS-AA.

Atom type	ε (kJ mol^{-1})	σ (Å)	q (e)
Choline Chloride			
Cl	0.80	4.0	-1.00000
N	0.70	3.2	-0.15456
CM	0.80	3.7	0.10974
CE	0.80	3.7	0.07411
HM	0.00	0.0	0.05244
CT	0.80	3.7	0.16201
HE	0.00	0.0	0.05244
HT	0.00	0.0	0.05244
OH	0.65	3.1	-0.31260
HO	0.00	0.0	0.22008
Glycerol			
CC	0.80	3.5	0.17000
CG	0.80	3.5	0.10700
O	0.65	3.1	-0.62500
OC	0.65	3.1	-0.62500
H	0.00	0.0	0.39200
HG	0.00	0.0	0.06300

Table S2: Intramolecular bond distance (Å) and bond-angle (°) constraints used to define the basic structure of the components in the initial EPSR simulation model

Bond length (Å)		Bond Angle (°)	
Choline Chloride			
CM–HM	1.08	HM–CM–HM	108.50
CM–N	1.51	HM–CM–N	108.50
N–CE	1.56	CM–N–CM	108.50
CE–HE	1.08	CM–N–CE	110.00
CE–CT	1.46	N–CE–HE	108.50
CT–HT	1.08	N–CE–CT	114.60
CT–OH	1.44	HE–CE–HE	108.50
OH–HO	0.97	HE–CE–CT	108.50
		CE–CT–HT	108.50
		CE–CT–OH	112.60
		HT–CT–HT	108.50
		OH–CT–HT	108.50
		CT–OH–HO	118.00
Glycerol			
O–CG	1.45	CG–O–H	109.90
O–H	0.97	CC–OC–H	108.30
OC–H	0.97	O-CG–CC	108.88
OC–CC	1.45	CC–CG–HG	110.17
CG–CC	1.54	O–CG–HG	109.51
CC–HG	1.08	HG–CG–HG	108.57
CG–HG	1.08	CG–CC–CG	111.20
		OC–CC-CG	108.72
		CG–CC–HG	109.61
		OC–CC–HG	108.96

Table S3: Dynamic viscosity (cP) as a function of temperature (°C) for $\chi_{ChCl} = 0.33$ and $\chi_{ChCl} = 0.5$

Temperature (°C)	$\chi_{ChCl} = 0.33$ / cP	$\chi_{ChCl} = 0.5$ / cP
20	352	466
25	257	345
30	193	262
35	148	204
40	114	161
45	89.2	128
50	70.8	102
55	56.9	82.2
60	49.9	67.9

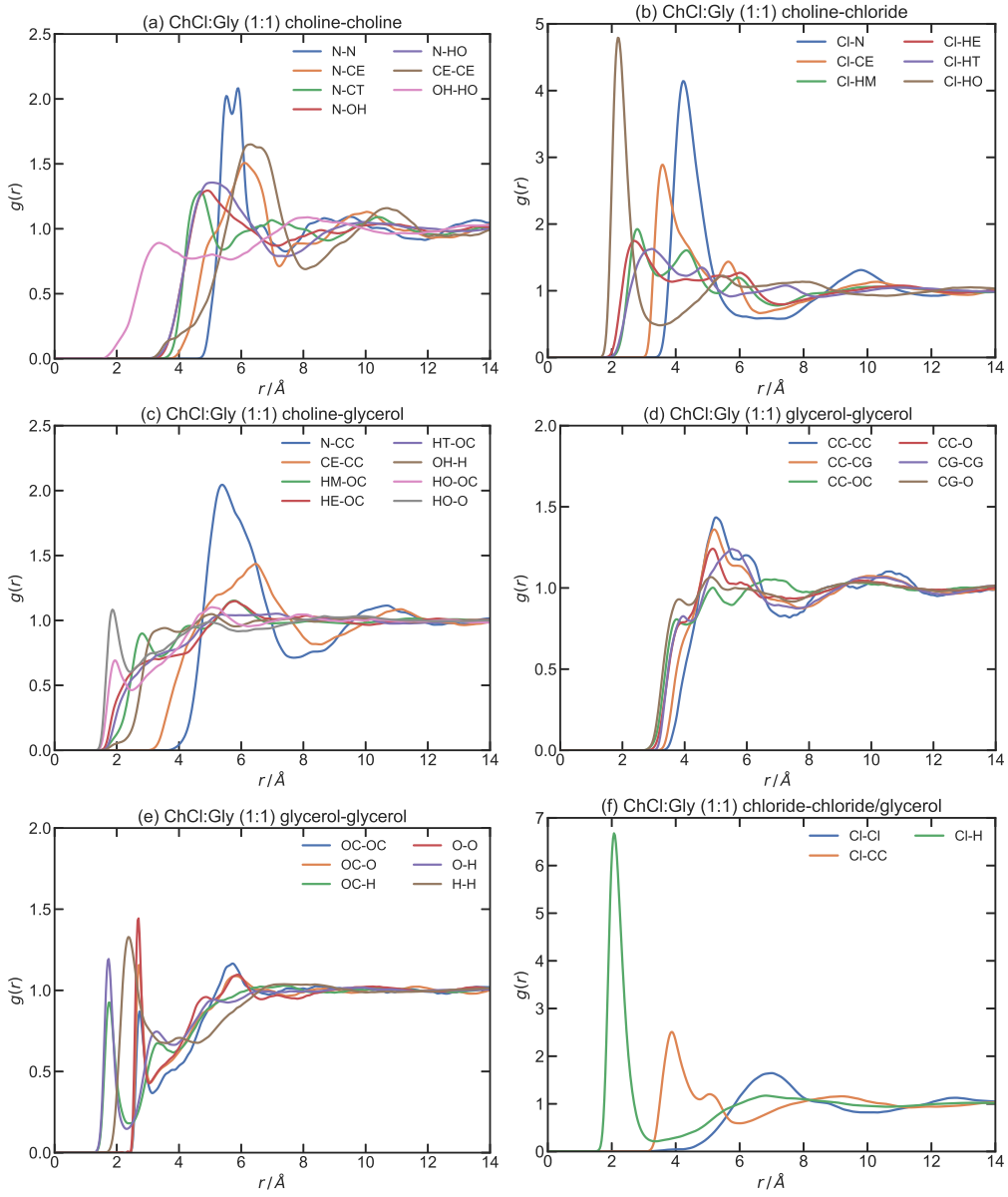

Figure S2: Atom-centred pRDFs for ChCl:Gly ($\chi_{ChCl} = 0.50$)