

“Micro- and mesoscopic structural features of a bio-based choline-amino acid ionic liquid.” By Olga Russina* , Serena De Santis, Lorenzo Gontrani

Supplementary information

Partial charges for the two residues NLE and COL.

Coline

O1 -0.602013
H1 0.445412
C1 0.261529
H2 0.013838
H3 0.013838
C2 -0.056046
H4 0.100214
H5 0.100214
N1 0.190230
C4 -0.306978
H9 0.161524
H10 0.161524
H11 0.161524
C5 -0.306978
H12 0.161524
H13 0.161524
H14 0.161524
C3 -0.306978
H6 0.161524
H7 0.161524
H8 0.161524

NLE

O1 -0.688904
C1 0.569776
O2 -0.688904
C2 0.453658
N1 -1.013086
H1 0.316121
H2 0.316121
H3 -0.051937
C3 -0.074454
H4 -0.033798
H5 -0.033798
C4 -0.056613
H6 0.015047
H7 0.015047
C5 0.124058
H8 -0.026260
H9 -0.026260
C6 -0.213882
H10 0.032689
H11 0.032689
H12 0.032689

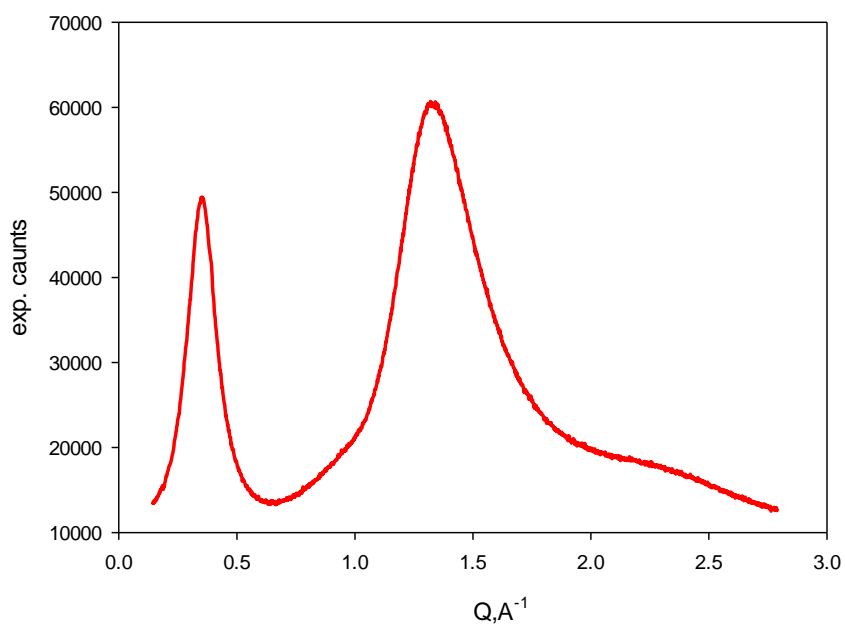


Fig 1. Diffraction data of [cho][nle] collected on x-ray diffractometer ($\lambda=0.1541 \text{ \AA}$) show evidently the presence of low Q-peak at around 0.35 \AA^{-1} .