

Supplementary information (SI):

Rotational dynamics of diammonium cations in lead bromide composites investigated by quasi-elastic neutron scattering

Kanming Shi,^a Lorenzo Malavasi,^b Fanni Juranyi^c and Maths Karlsson^{*a}

^a Department of Chemistry and Chemical Engineering, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

^b Department of Chemistry, University of Pavia & INSTM, Viale Taramelli 16, 27100 Pavia, Italy

^c Laboratory for Neutron Scattering and Imaging, PSI Center for Neutron and Muon Sciences, Forschungsstrasse 111, 5232 Villigen, Switzerland

*Email: maths.karlsson@chalmers.se

Contents

S1 Energy integrated neutron scattering data	S2
S2 Additional $S(Q, E)$ data and fits	S3
S2.1 $S(Q, E)$ of (1,3-PDA)PbBr ₄	S3
S2.2 $S(Q, E)$ of (1,3-XDA) ₂ PbBr ₆	S4
S2.3 $S(Q, E)$ of (1,4-PDA)PbBr ₄	S5
S2.4 $S(Q, E)$ of (1,4-XDA)PbBr ₄	S5
S3 Additional EISF models and fits	S6

S1 Energy integrated neutron scattering data

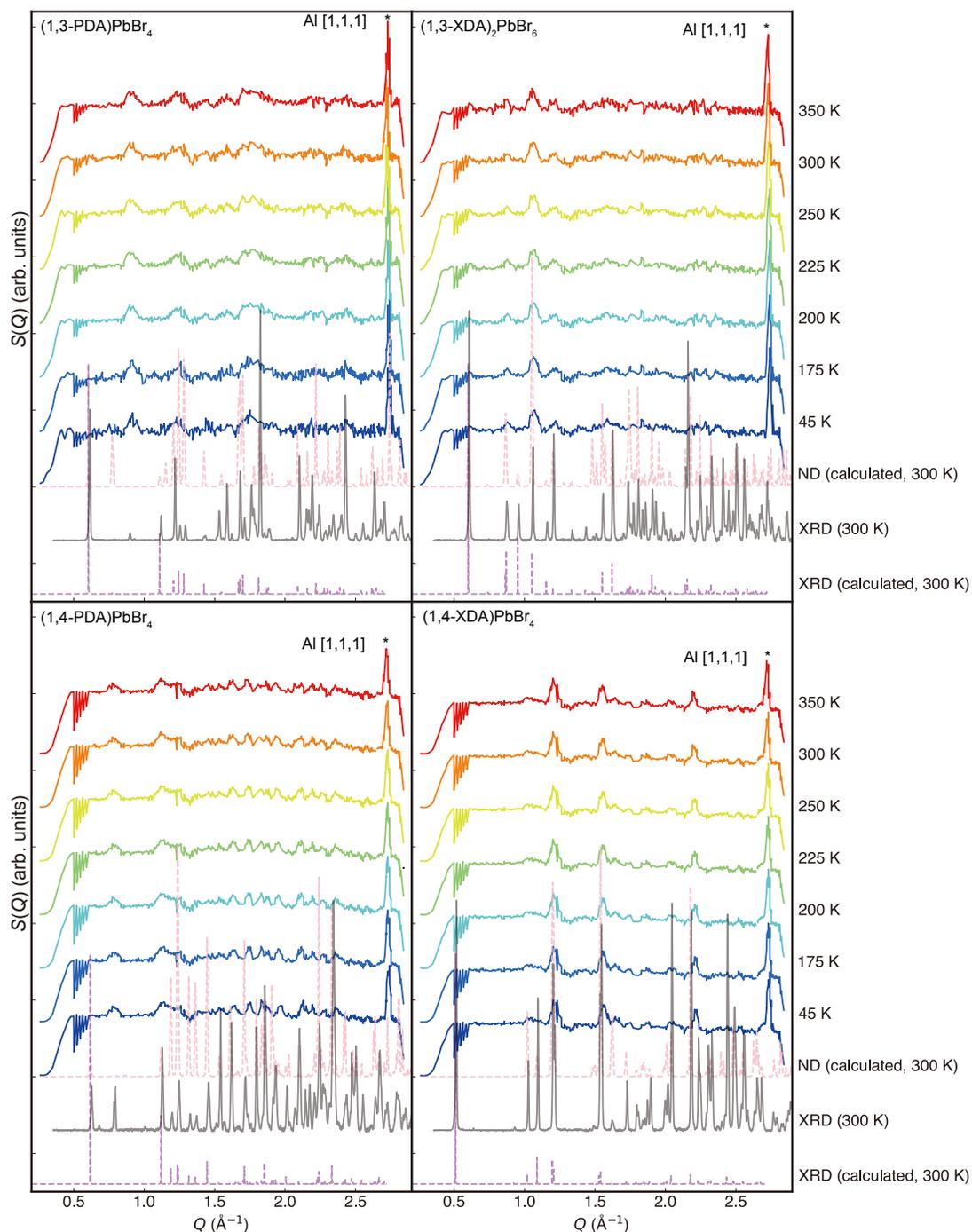


Fig. S1 Variable temperature $S(Q)$ data for 2D MHPs (1,3-PDA) PbBr_4 , (1,4-PDA) PbBr_4 , and (1,4-XDA) PbBr_4 , and 0D perovskitoid (1,3-XDA) $_2\text{PbBr}_6$. The peak marked with an asterisk at approximately 2.7 \AA^{-1} originates from the aluminum sample cell. The pink dashed lines are the calculated neutron diffraction (ND) pattern, the grey lines are the XRD data, and the purple dashed lines are the calculated XRD patterns.

S2 Additional $S(Q, E)$ data and fits

S2.1 $S(Q, E)$ of (1,3-PDA)PbBr₄

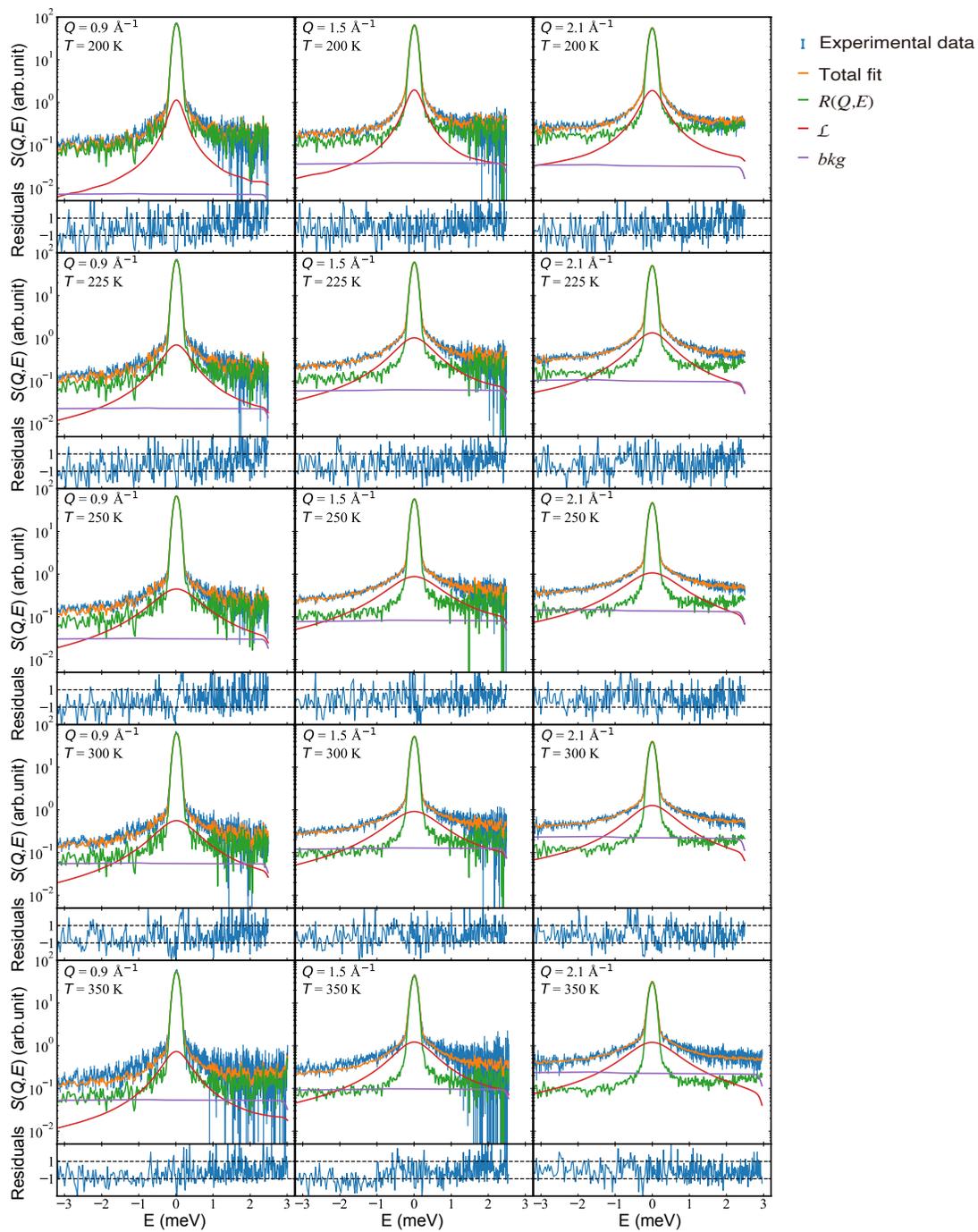


Fig. S2 $S(Q, E)$ with fits for (1,3-PDA)PbBr₄.

S2.2 $S(Q, E)$ of $(1,3\text{-XDA})_2\text{PbBr}_6$

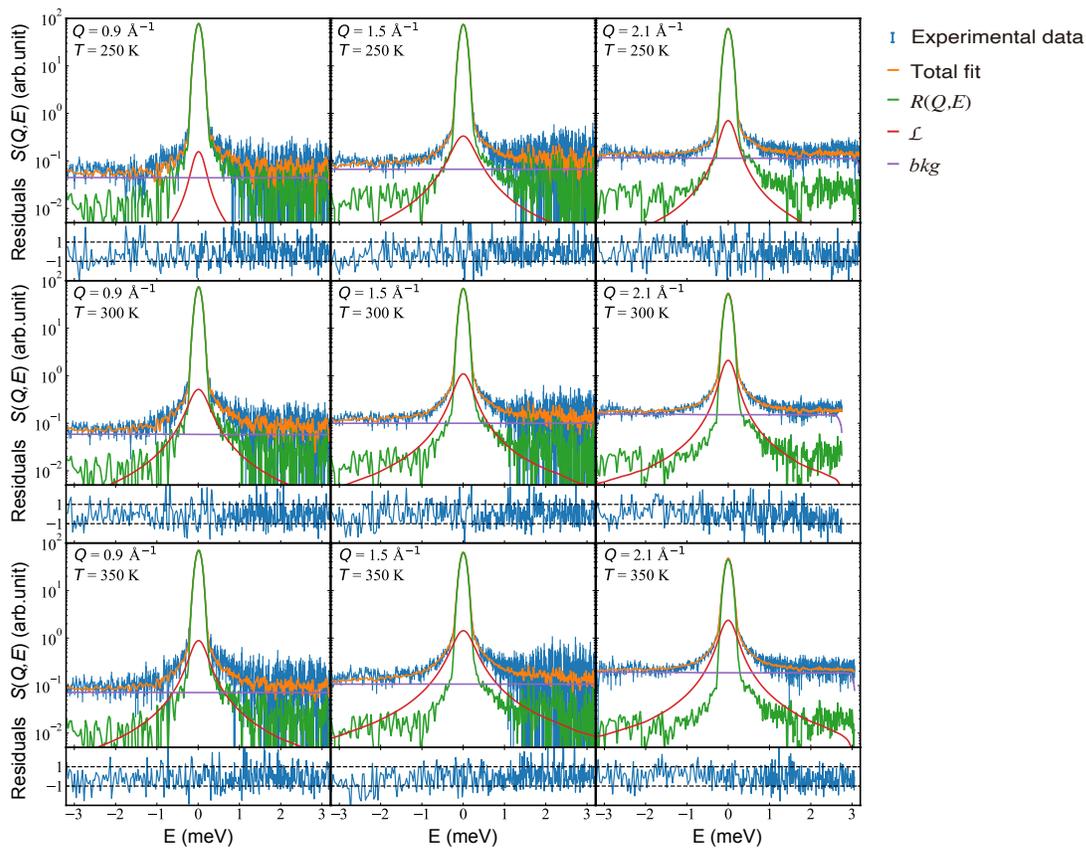


Fig. S3 $S(Q, E)$ with fits for $(1,3\text{-XDA})_2\text{PbBr}_6$.

S2.3 $S(Q, E)$ of (1,4-PDA)PbBr₄

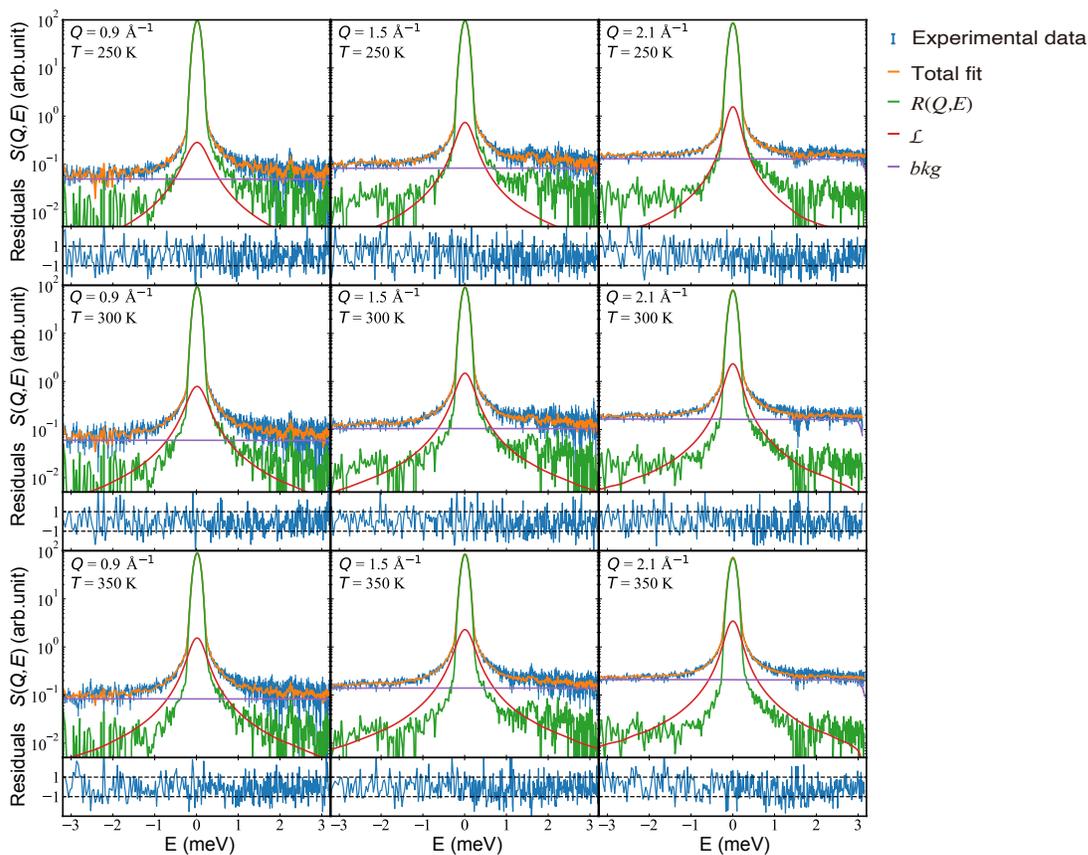


Fig. S4 $S(Q, E)$ with fits for (1,4-PDA)PbBr₄.

S2.4 $S(Q, E)$ of (1,4-XDA)PbBr₄

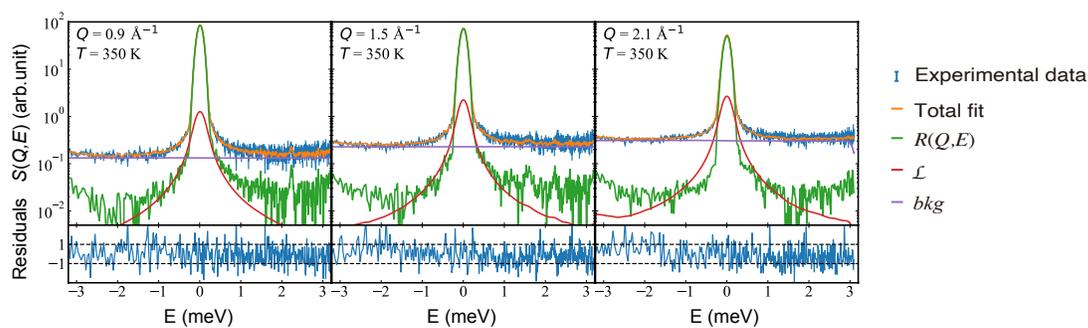
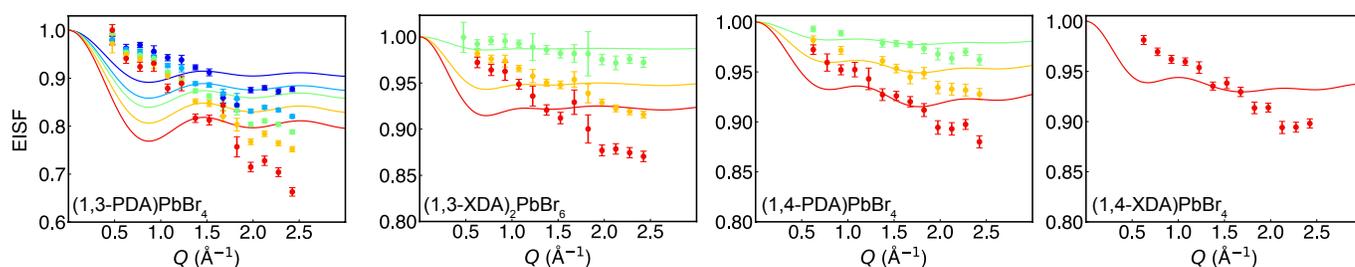


Fig. S5 $S(Q, E)$ with fits for (1,4-XDA)PbBr₄.

S3 Additional EISF models and fits

(a) C_2 rotational diffusion around its short molecular axis



(b) C_3 rotational diffusion of the $-\text{NH}_3$ group together with C_2 rotational diffusion of the phenylene ring

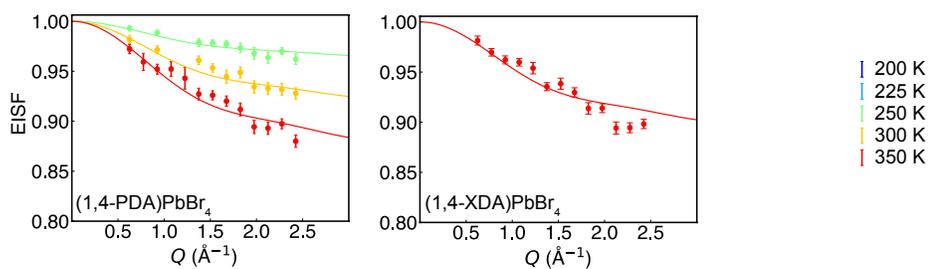


Fig. S6 EISF fitting results with (a) C_2 rotational diffusion of the whole organic cation around its short molecular axis, and (b) C_3 rotational diffusion of the $-\text{NH}_3$ group together with C_2 rotational diffusion of the phenylene ring.