

Figure A1 Fit of {NEAT(4)} D<sub>2</sub>O spectra,  $\lambda_0 = 5.1 \text{ \AA}$ ,  $\Delta E = 90 \mu\text{eV}$ , low  $Q$  region. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “D2O” and “EC” are the QENS components due to D<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by D<sub>2</sub>O.

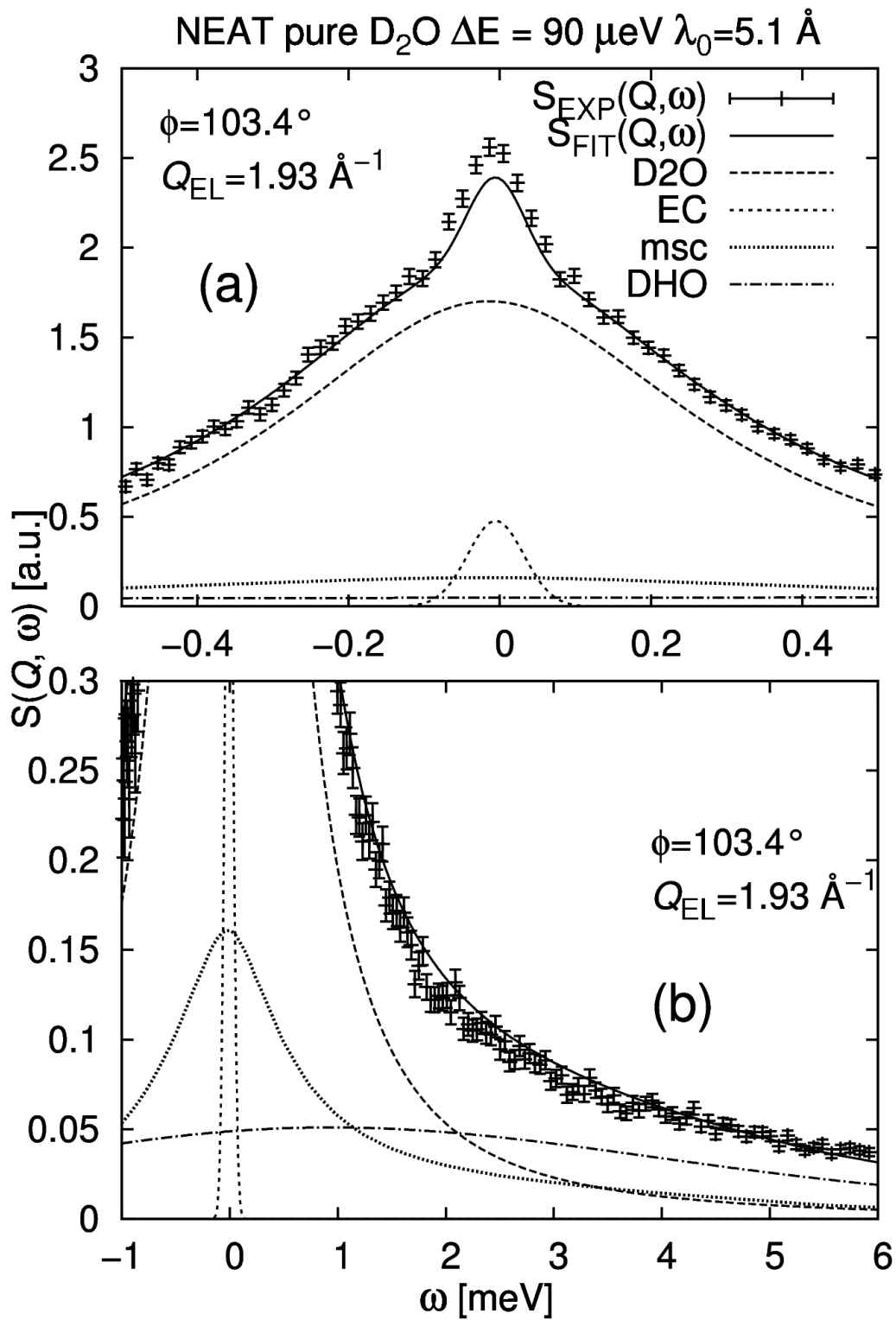


Figure A2 Fit of {NEAT(4)} D<sub>2</sub>O spectra,  $\lambda_0 = 5.1 \text{ \AA}$ ,  $\Delta E = 90 \mu\text{eV}$ , high  $Q$  region. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “D2O” and “EC” are the QENS components due to D<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by D<sub>2</sub>O.

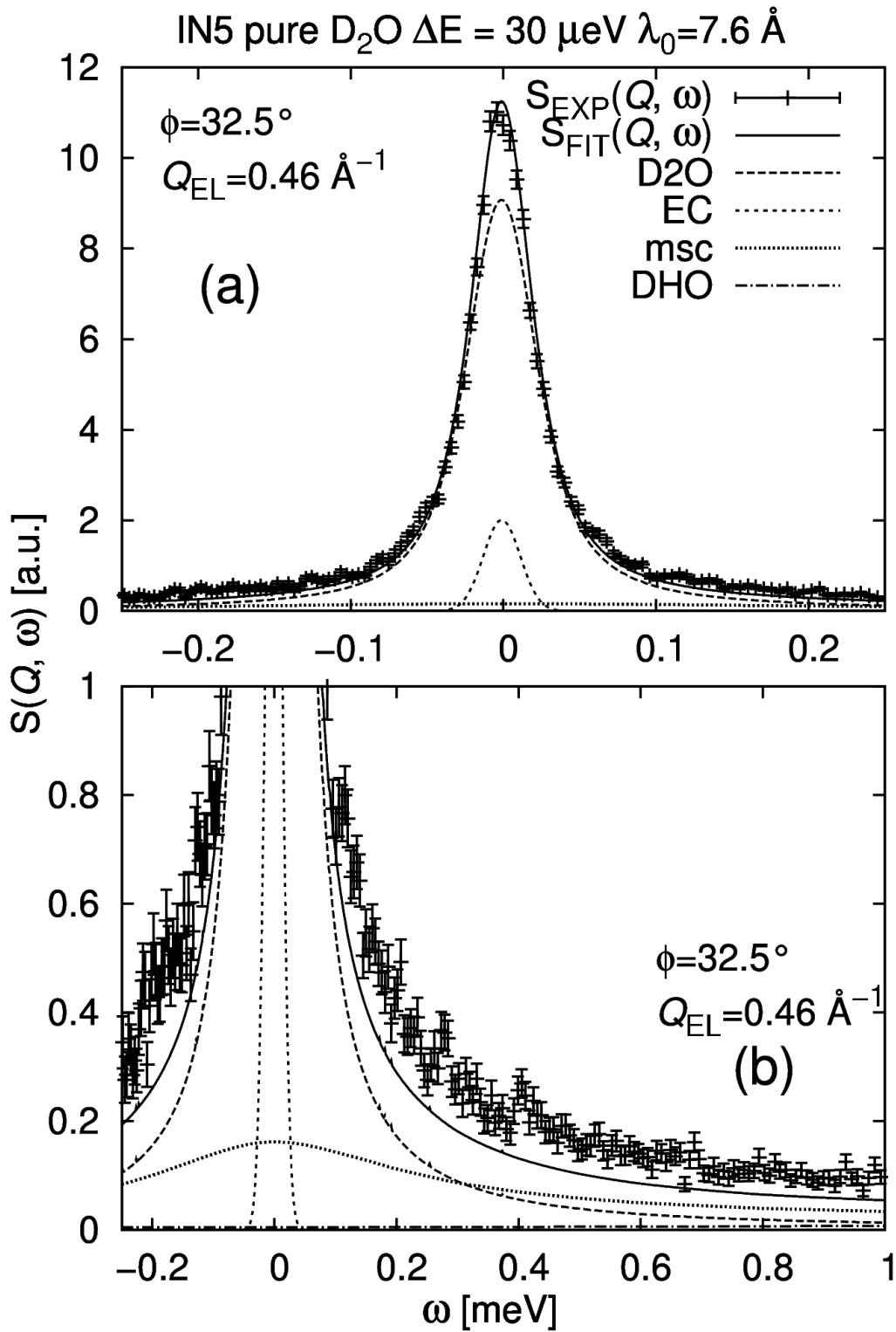


Figure A3 Fit of {IN5(1)} D<sub>2</sub>O spectra,  $\lambda_0 = 7.6 \text{ \AA}$ ,  $\Delta E = 30 \mu\text{eV}$ , low  $Q$  region. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “D2O” and “EC” are the QENS components due to D<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by D<sub>2</sub>O.

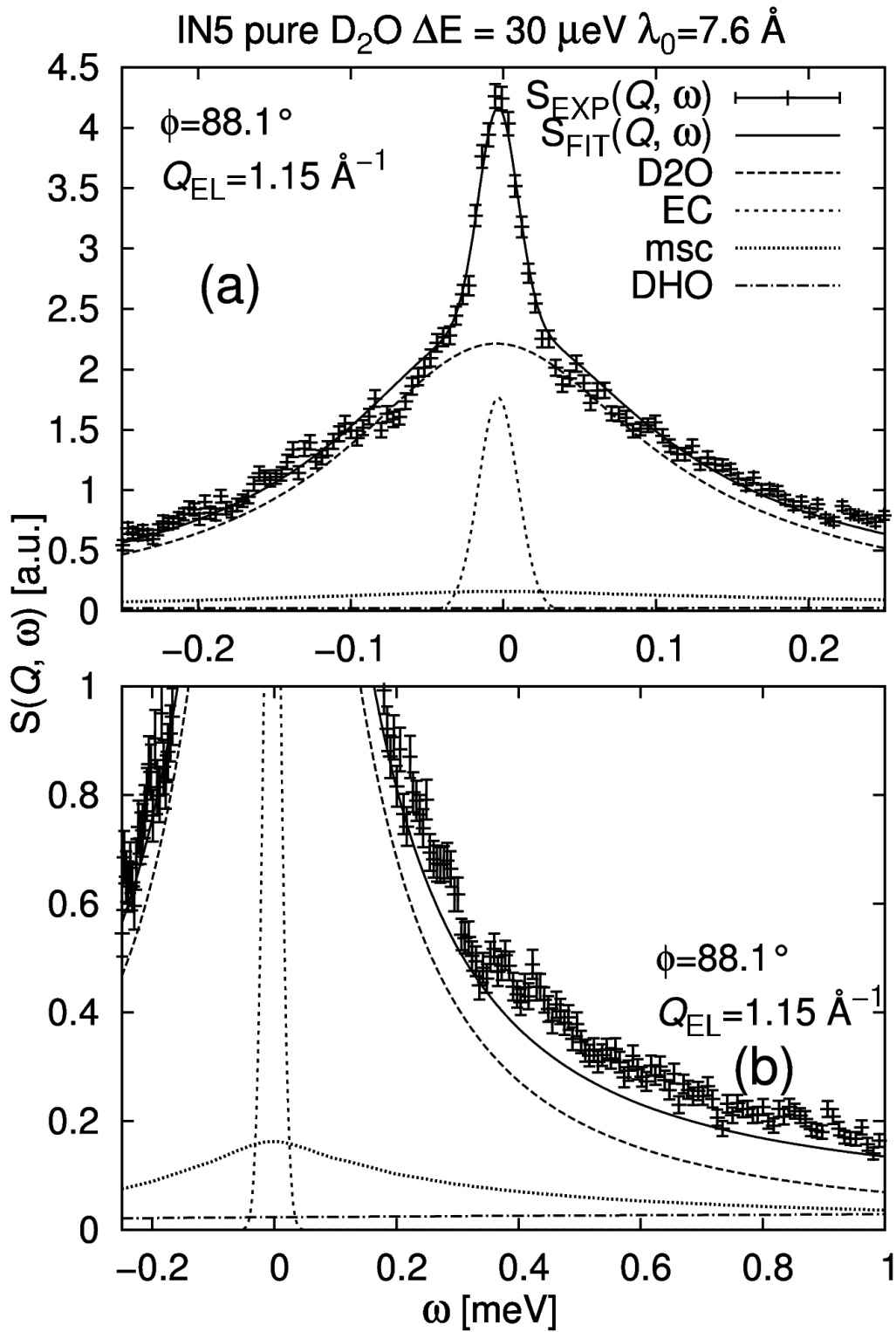


Figure A4 Fit of {IN5(1)} D<sub>2</sub>O spectra,  $\lambda_0 = 7.6 \text{ \AA}$ ,  $\Delta E = 30 \mu\text{eV}$ , high  $Q$  region. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “D2O” and “EC” are the QENS components due to D<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by D<sub>2</sub>O.

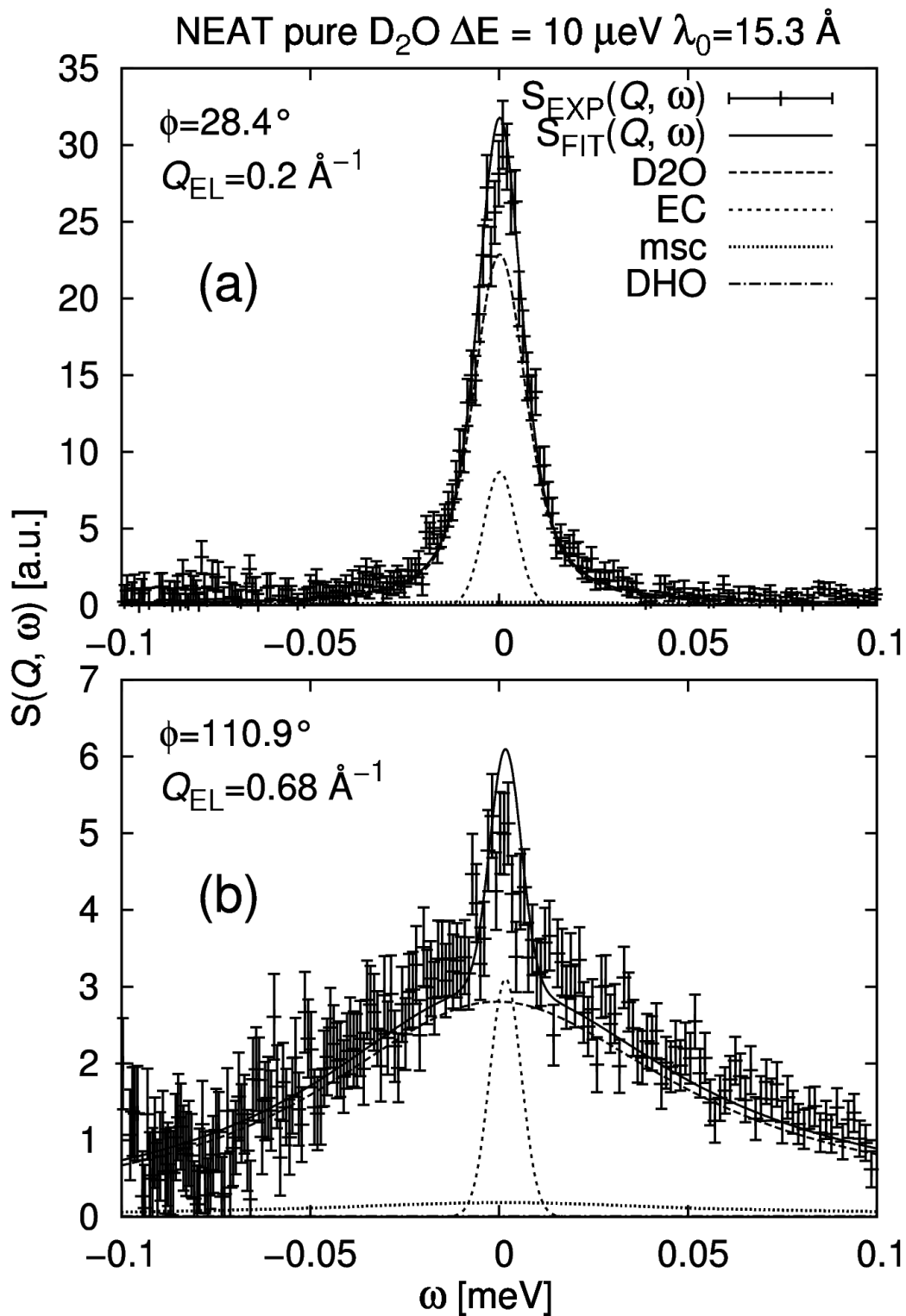


Figure A5 Fit of {NEAT(3)} D<sub>2</sub>O spectra,  $\lambda_0 = 15.3 \text{ \AA}$ ,  $\Delta E = 10 \mu\text{eV}$ . The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “D2O” and “EC” are the QENS components due to D<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by D<sub>2</sub>O.

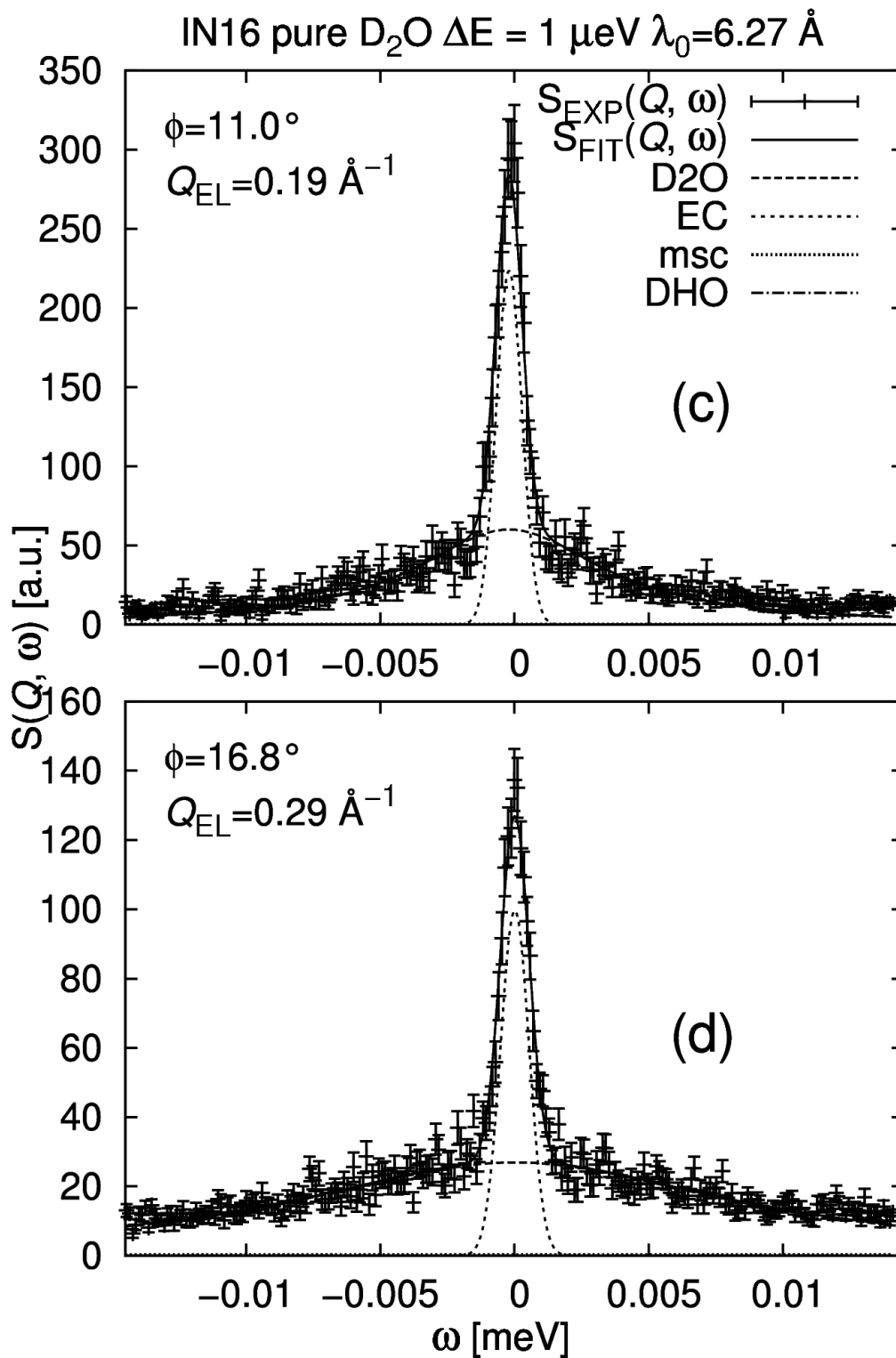


Figure A6 Fit of {IN16} D<sub>2</sub>O spectra,  $\lambda_0 = 6.27 \text{ \AA}$ ,  $\Delta E = 1 \mu\text{eV}$ . The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “D2O” and “EC” are the QENS components due to D<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by D<sub>2</sub>O.

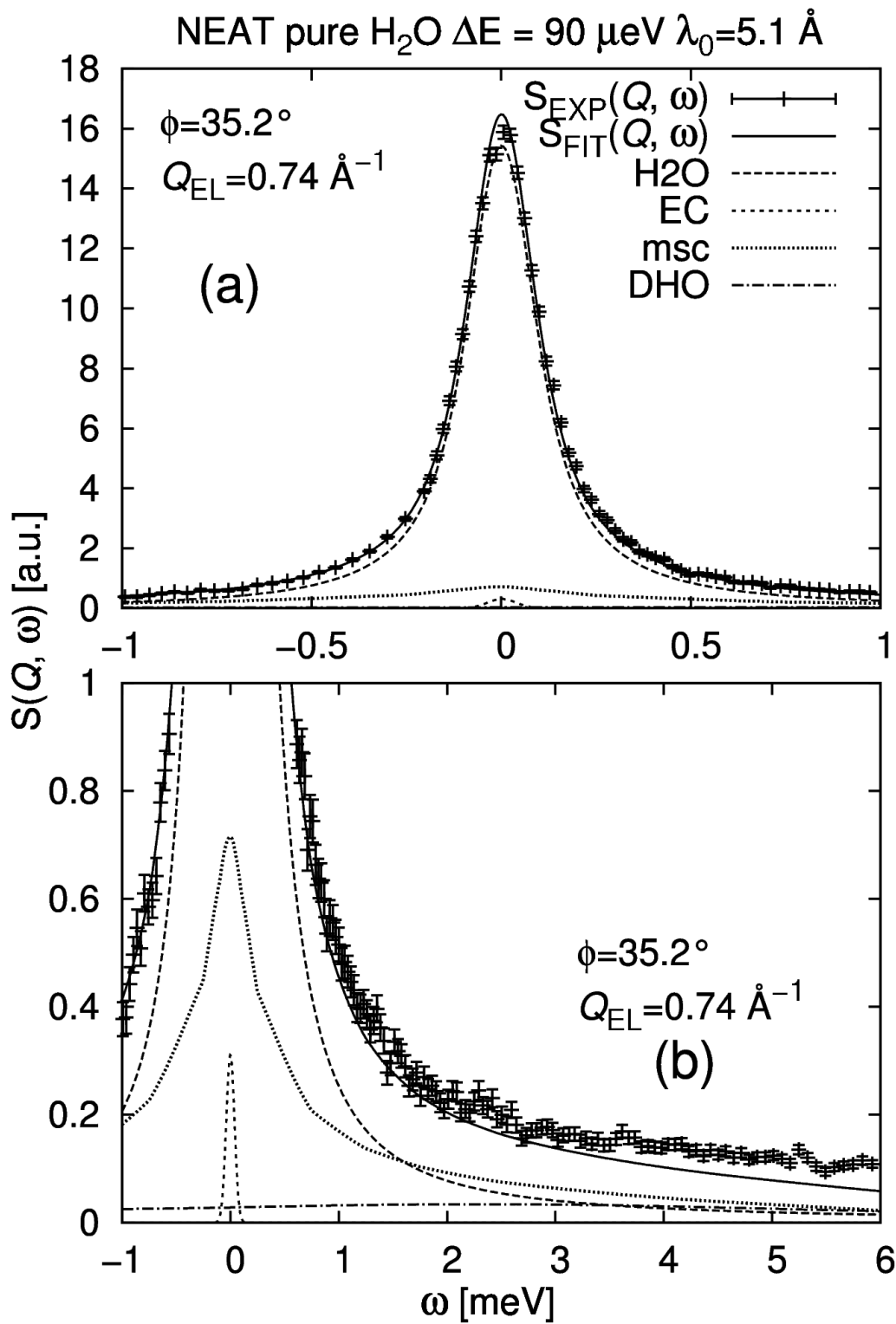


Figure A7 Fit of {NEAT(2)} H<sub>2</sub>O spectra,  $\lambda_0 = 5.1 \text{ \AA}$ ,  $\Delta E = 90 \mu\text{eV}$ , low  $Q$  region. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “H<sub>2</sub>O” and “EC” are the QENS components due to H<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by H<sub>2</sub>O.

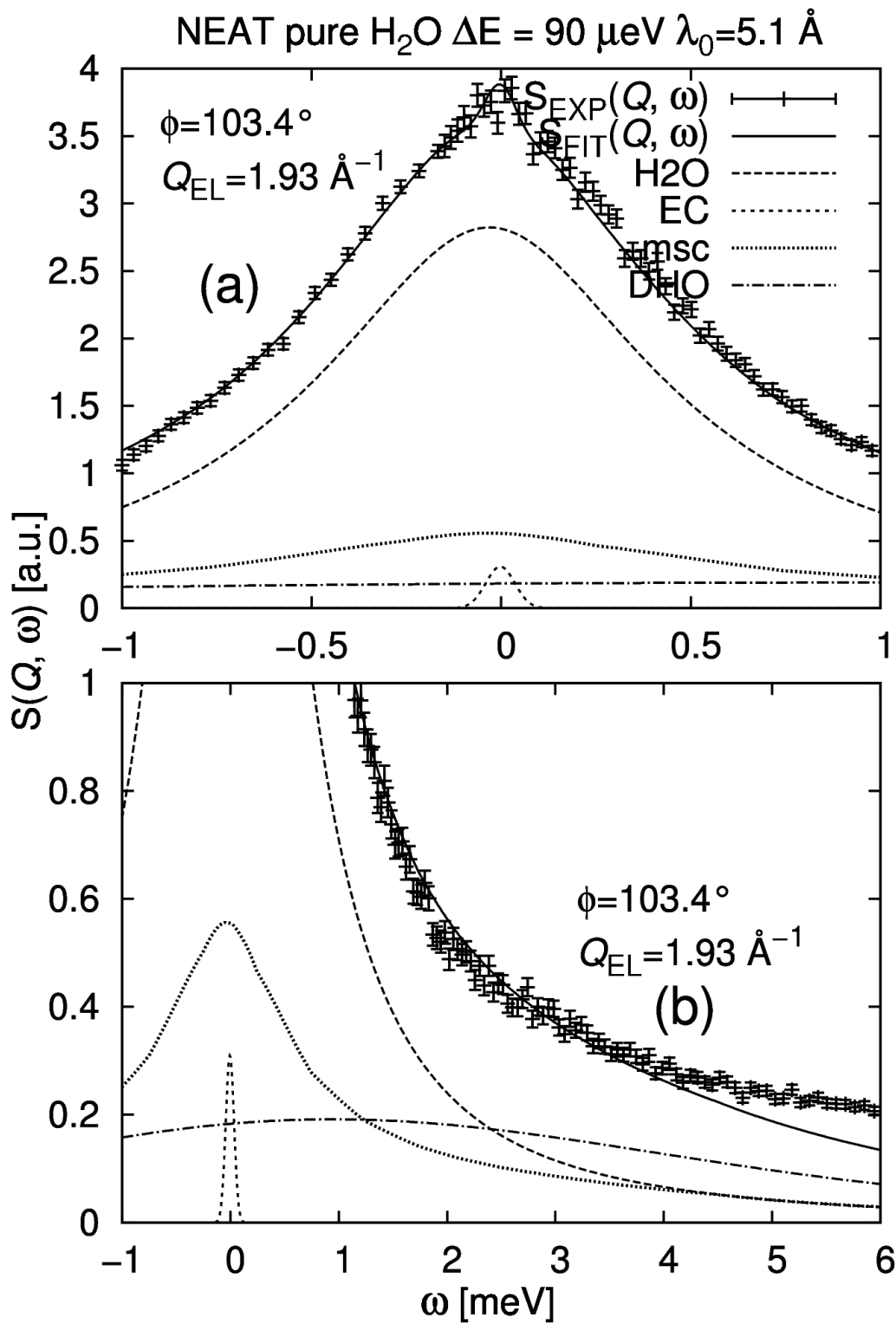


Figure A8 Fit of {NEAT(2)} H<sub>2</sub>O spectra,  $\lambda_0 = 5.1 \text{ \AA}$ ,  $\Delta E = 90 \mu\text{eV}$ , high  $Q$  region. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “H<sub>2</sub>O” and “EC” are the QENS components due to H<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by H<sub>2</sub>O.



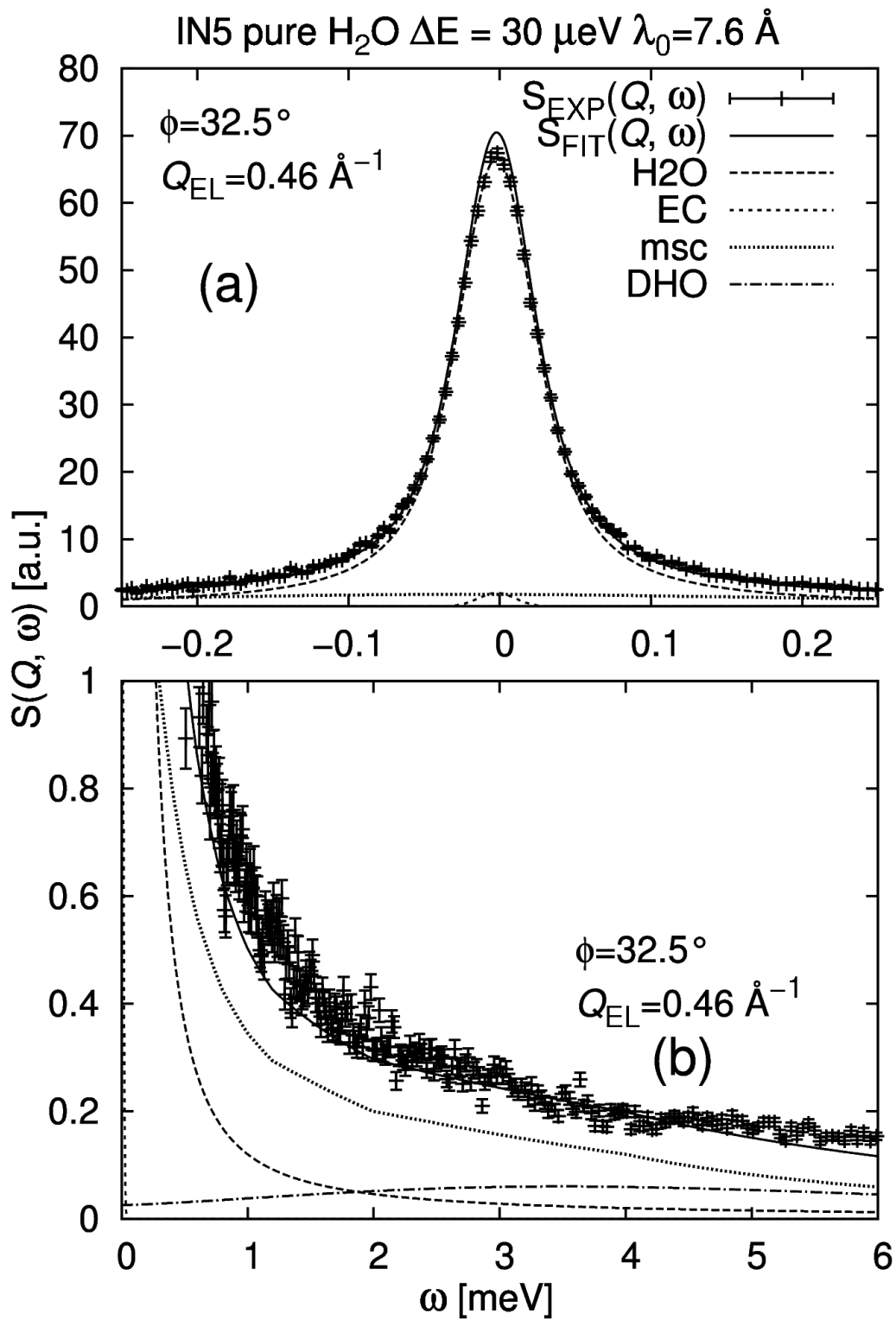


Figure A9 Fit of {IN5(2)} H<sub>2</sub>O spectra,  $\lambda_0 = 7.6 \text{ \AA}$ ,  $\Delta E = 30 \mu\text{eV}$ , low  $Q$  region. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “H<sub>2</sub>O” and “EC” are the QENS components due to H<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by H<sub>2</sub>O.

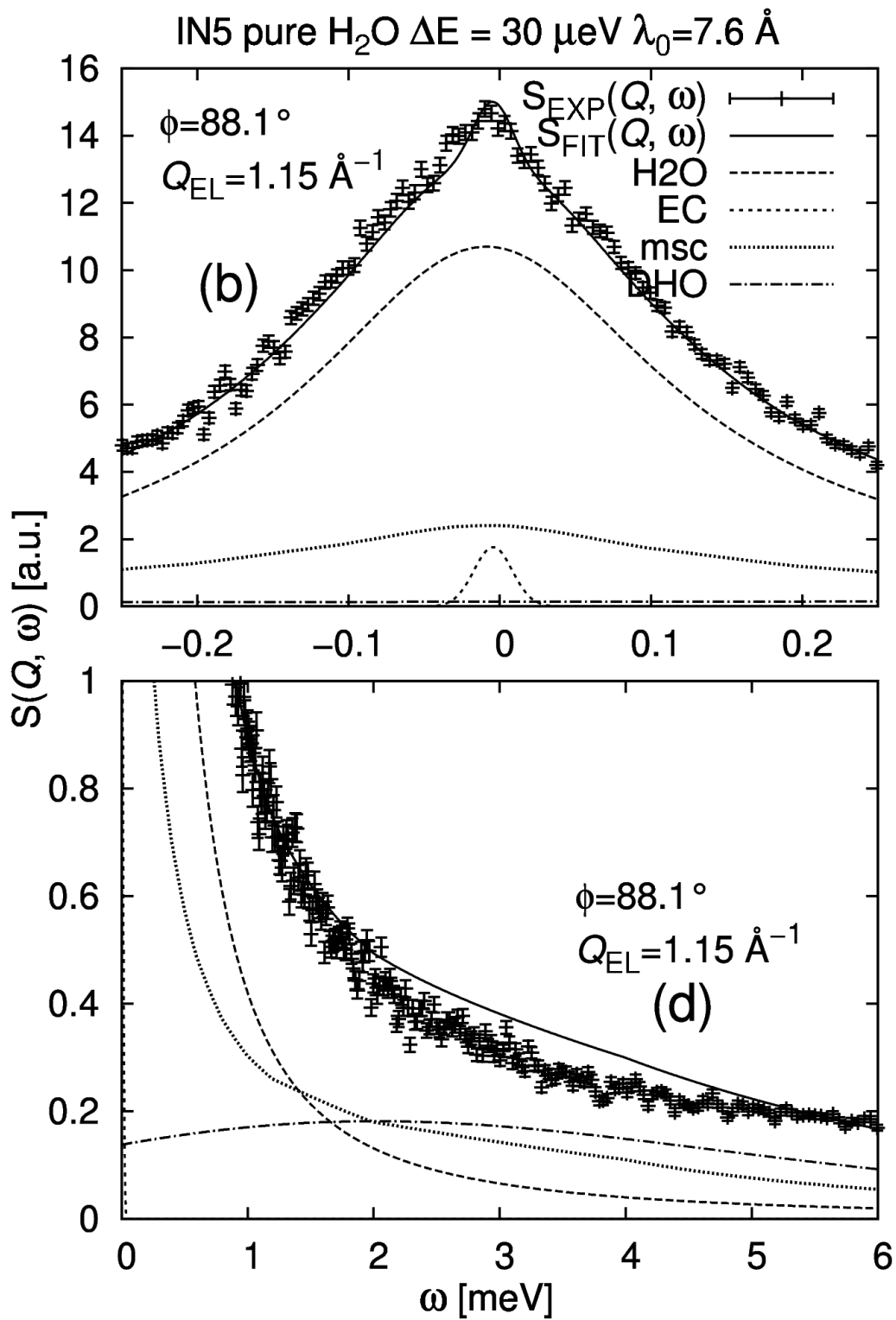


Figure A10 Fit of {IN5(2)} H<sub>2</sub>O spectra,  $\lambda_0=7.6 \text{ \AA}$ ,  $\Delta E=30 \mu\text{eV}$ , high  $Q$  region. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “H<sub>2</sub>O” and “EC” are the QENS components due to H<sub>2</sub>O and the sample container scattering, respectively. “msc” is the multiple scattering and “DHO” represents the inelastic scattering by H<sub>2</sub>O.

Appendix B Examples of fitted QENS spectra of DIMEB solutions in D<sub>2</sub>O

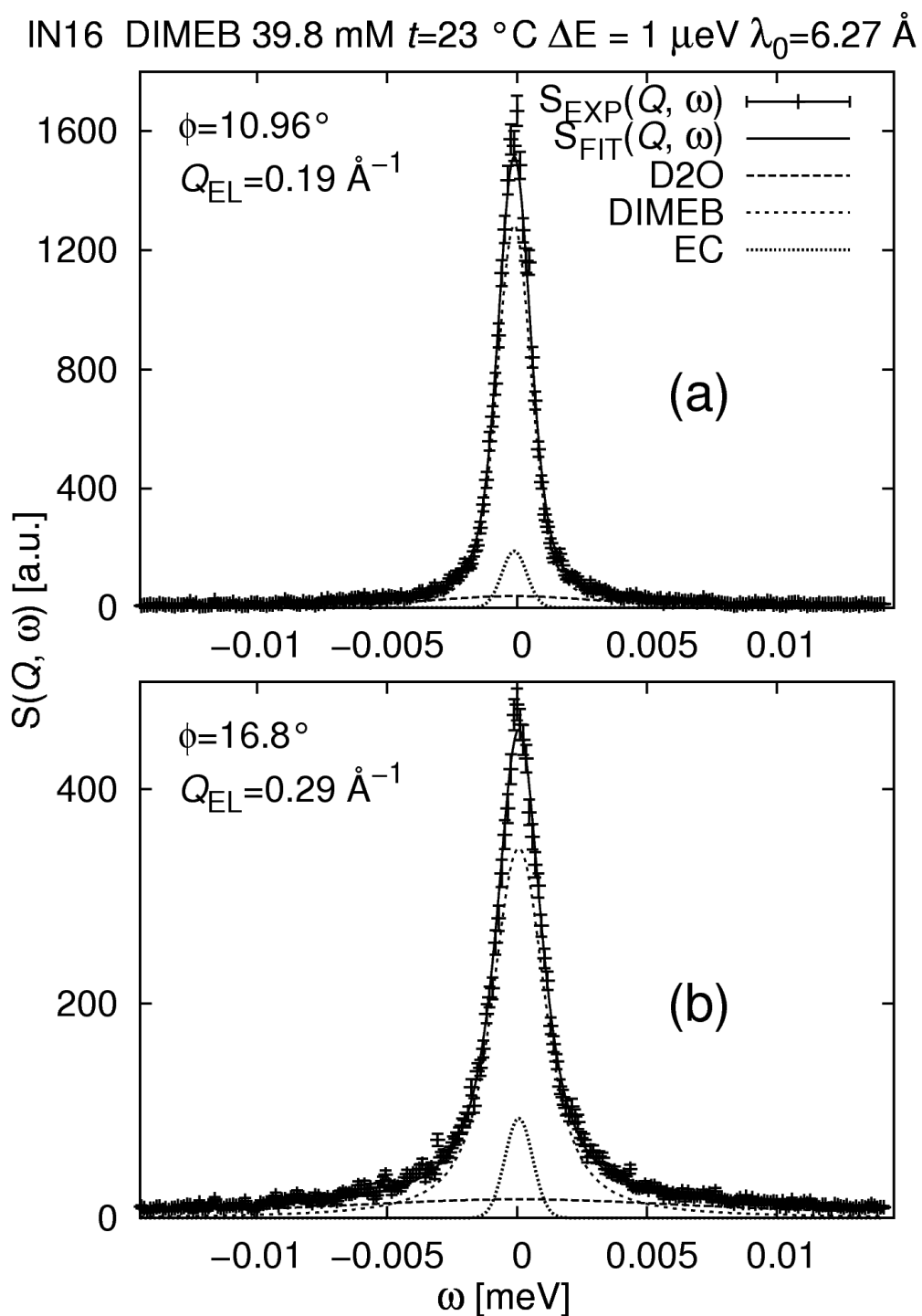


Figure B1 Examples of the fit of the “standard solute model” to {IN16} spectra of DIMEB solutions in heavy water, 39.8 mM,  $\phi=10.96^\circ$  and  $16.80^\circ$ . The spectra for two scattering angles,  $10.96^\circ$  and  $16.80^\circ$ , are shown;  $D_{\text{r,SOL}}$  was fixed to zero. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “D<sub>2</sub>O”, “DIMEB” and “EC” are the QENS components due to D<sub>2</sub>O, DIMEB and the sample container scattering, respectively.

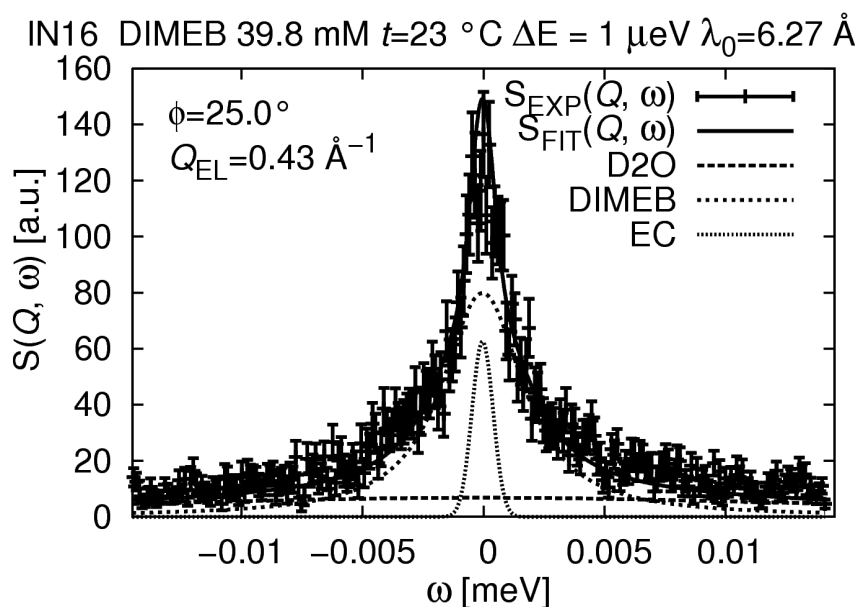


Figure B2 Example of the fit of the “standard solute model” to {IN16} spectra of DIMEB solutions in heavy water, 39.8 mM,  $\phi=25.0^\circ$ . The spectrum for the scattering angle  $25.0^\circ$  is shown;  $D_{\text{r,SOL}}$  was fixed to zero. Note: because of the fast increase of the spectral broadening with  $Q$ , the statistical accuracy is getting poorer with an increase in the scattering angle. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “D2O”, “DIMEB” and “EC” are the QENS components due to  $\text{D}_2\text{O}$ , DIMEB and the sample container scattering, respectively.

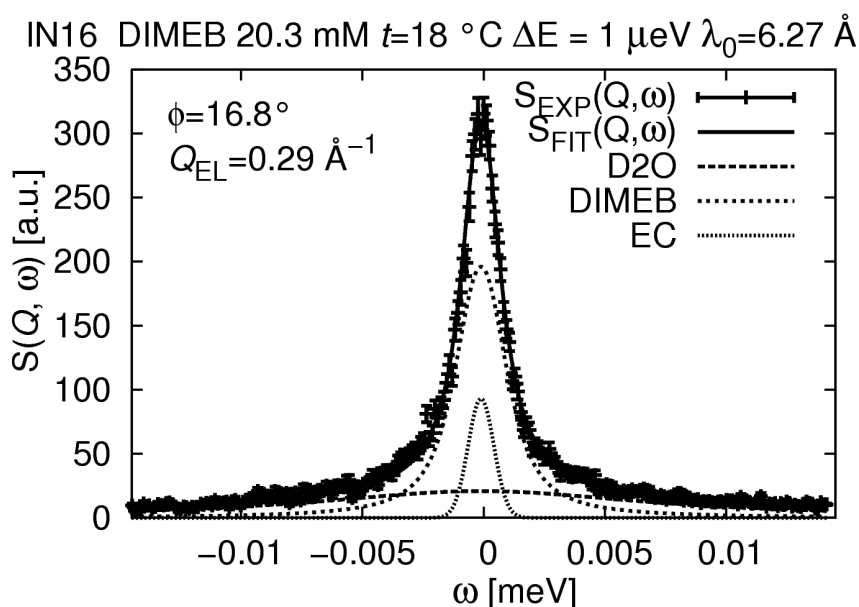


Figure B3 Example of the fit of the “standard solute model” to {IN16} spectra of DIMEB solutions in heavy water, 20.3 mM,  $\phi=16.8^\circ$ . The spectrum for the scattering angle  $16.8^\circ$  is shown;  $D_{\text{r,SOL}}$  was fixed to zero. Concentration of DIMEB here: 20.3 mM. The total fitted curve:  $S_{\text{FIT}}(Q, \omega)$ ; “D2O”, “DIMEB” and “EC” are the QENS components due to  $\text{D}_2\text{O}$ , DIMEB and the sample container scattering, respectively.

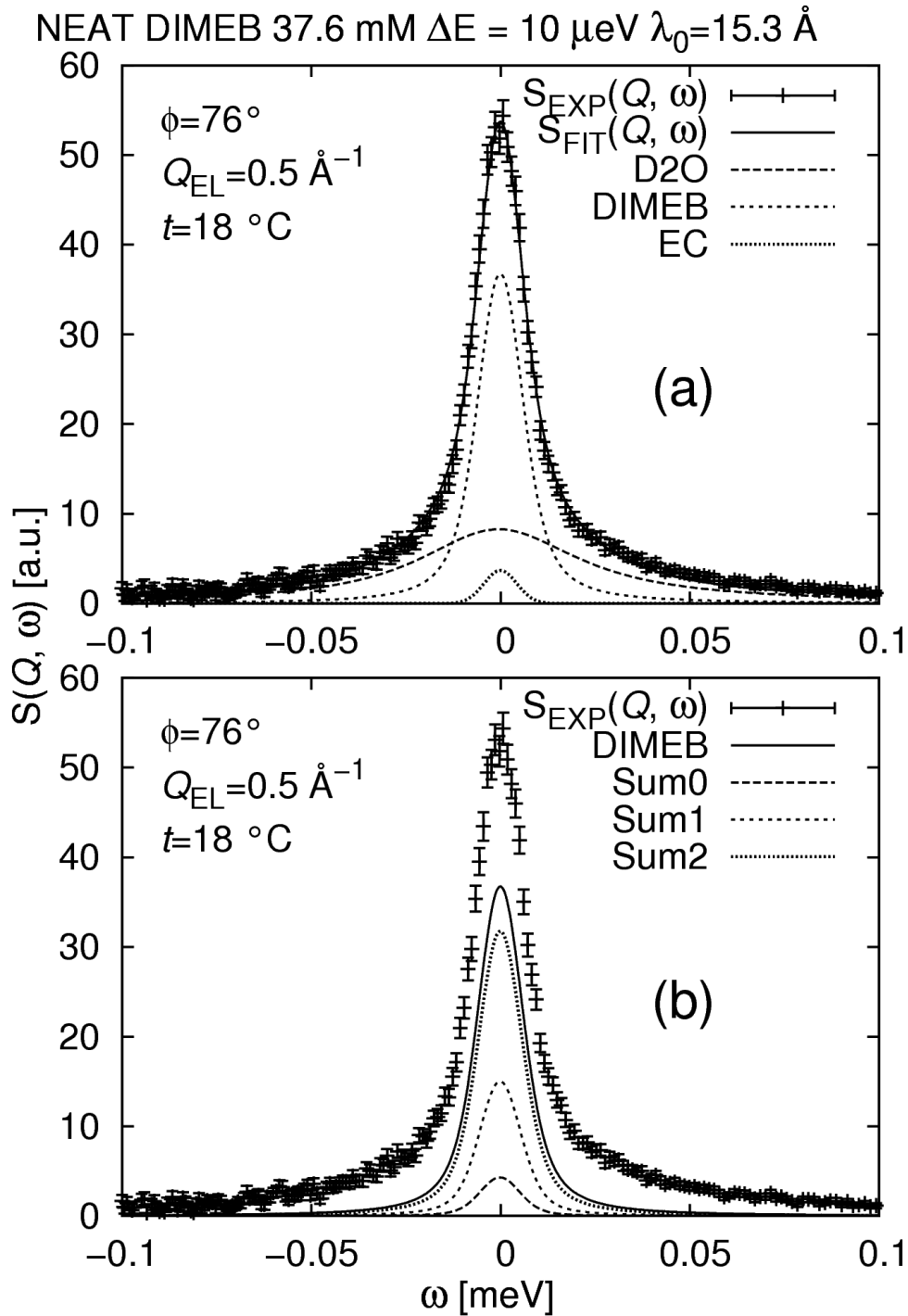


Figure B4 Examples of the fits of the “standard solute model” to the {NEAT(3)} spectra of DIMEB solutions in heavy water, 37.6 mM,  $\phi=76^\circ$ .  $D_{\text{TR SOL}}$  was fixed to the values found for DIMEB 39.8 mM, see Tab. 7.4. In (a):  $S_{\text{FIT}}(Q, \omega)$  is the total fitted curve; “D2O”, “DIMEB” and “EC” are the QENS components due to  $\text{D}_2\text{O}$ , DIMEB and the sample container scattering, respectively. In (b): the decomposition of the DIMEB scattering component, “DIMEB”, is shown. “Sum0” is the translational component (i.e.  $l=0$ ), “Sum1” is the sum of the components with  $l=0$  and 1, “Sum2” is the sum of the components with  $l=0, 1$  and 2.

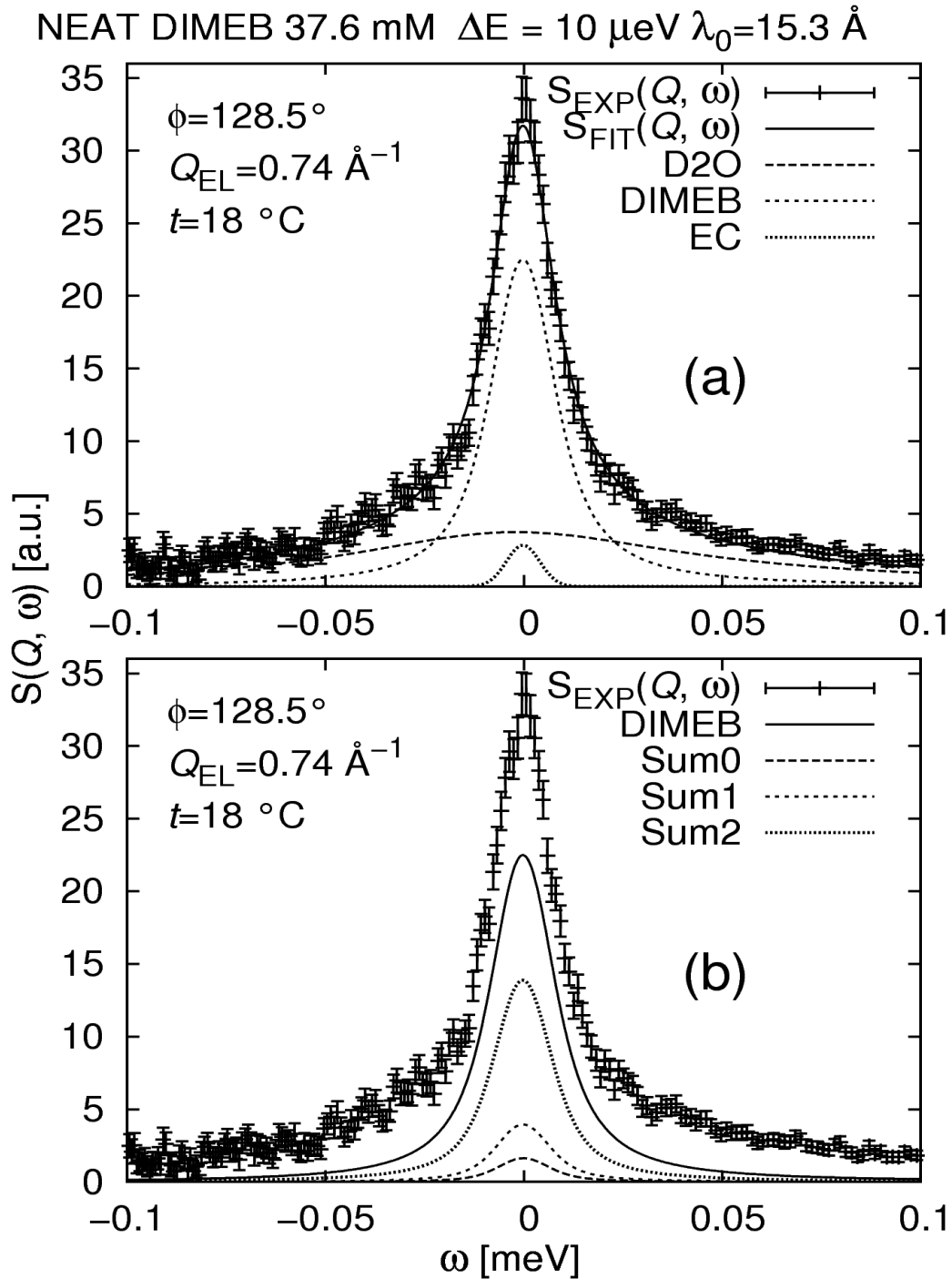


Figure B5 Examples of the fits of the “standard solute model” to the {NEAT(3)} spectra of DIMEB solutions in heavy water, 37.6 mM,  $\phi = 128.5^\circ$ .  $D_{\text{TR SOL}}$  was fixed to the values found for DIMEB 39.8 mM, see Tab. 7.4. In (a):  $S_{\text{FIT}}(Q, \omega)$  is the total fitted curve; “D2O”, “DIMEB” and “EC” are the QENS components due to D<sub>2</sub>O, DIMEB and the sample container scattering, respectively. In (b), the decomposition of the DIMEB scattering component, “DIMEB”, is shown. “Sum0” is the translational component (i.e.  $l=0$ ), “Sum1” is the sum of the components with  $l=0$  and 1, “Sum2” is the sum of the components with  $l=0, 1$  and 2.