Electronic Supplementary Material (ESI) for Faraday Discussions.
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Ultraintense, ultrashort pulse x-ray scattering in small molecules

Supplementary material

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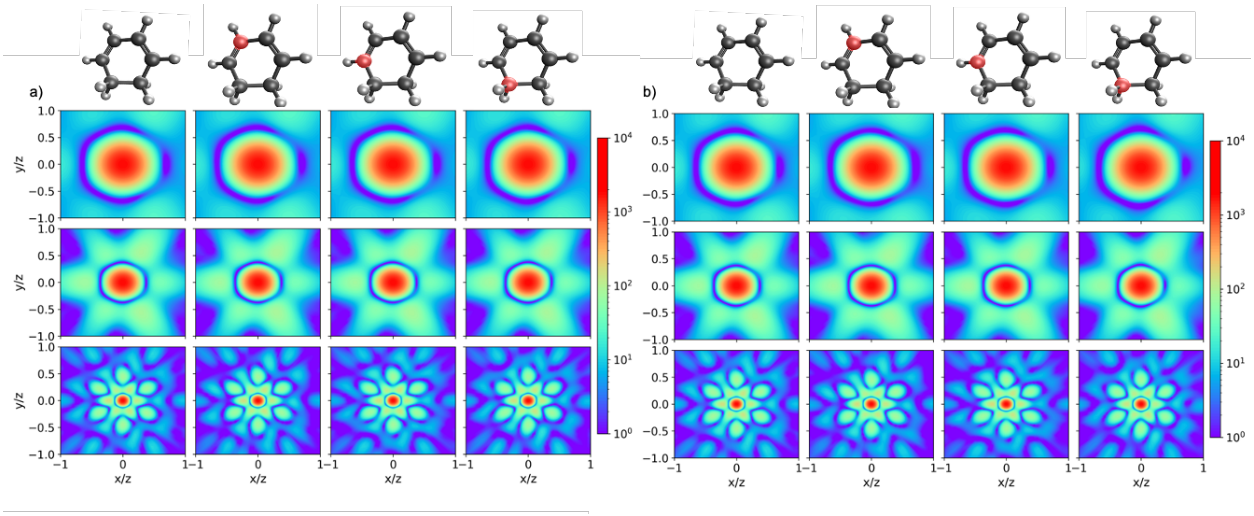

Figure S1: Detector images of the differential cross section for the coherent x-ray scattering of fixed-in-space 1-3-cyclohexadiene simulated by the HF method in a) and by DFT (B3LYP 6-311+G*), with optimised core hole states in b). The columns represent the electronic state and the rows the photon energy. The first column in both a) and b) is the neutral ground state and the next three are core ionised states, the carbon with the core hole is indicated in red at the top of each column. The first second and third rows show photon energies of 5.6, 9 and 24 keV respectively.

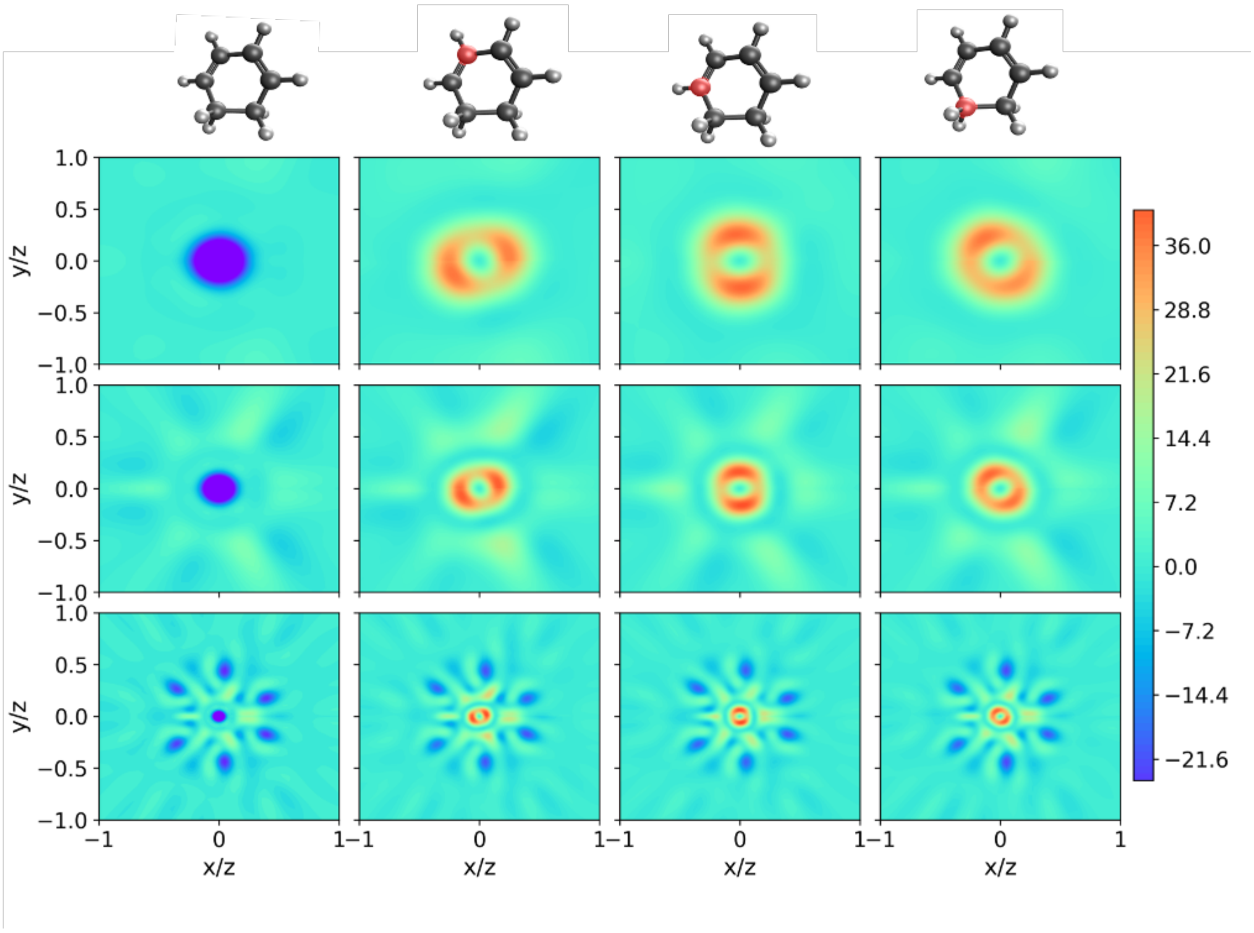

Figure S2: Comparisons of the coherent x-ray scattering calculations of 1-3-cyclohexadiene by difference between the HF(6-311+G*) and IAM. The first second and third rows show photon energies of 5.6, 9 and 24 keV respectively throughout. The first column in both a) and b) is the neutral ground state and the next three, are core ionised states. The carbon with the core hole is indicated in red at the top of each column. The ground state geometry is used throughout

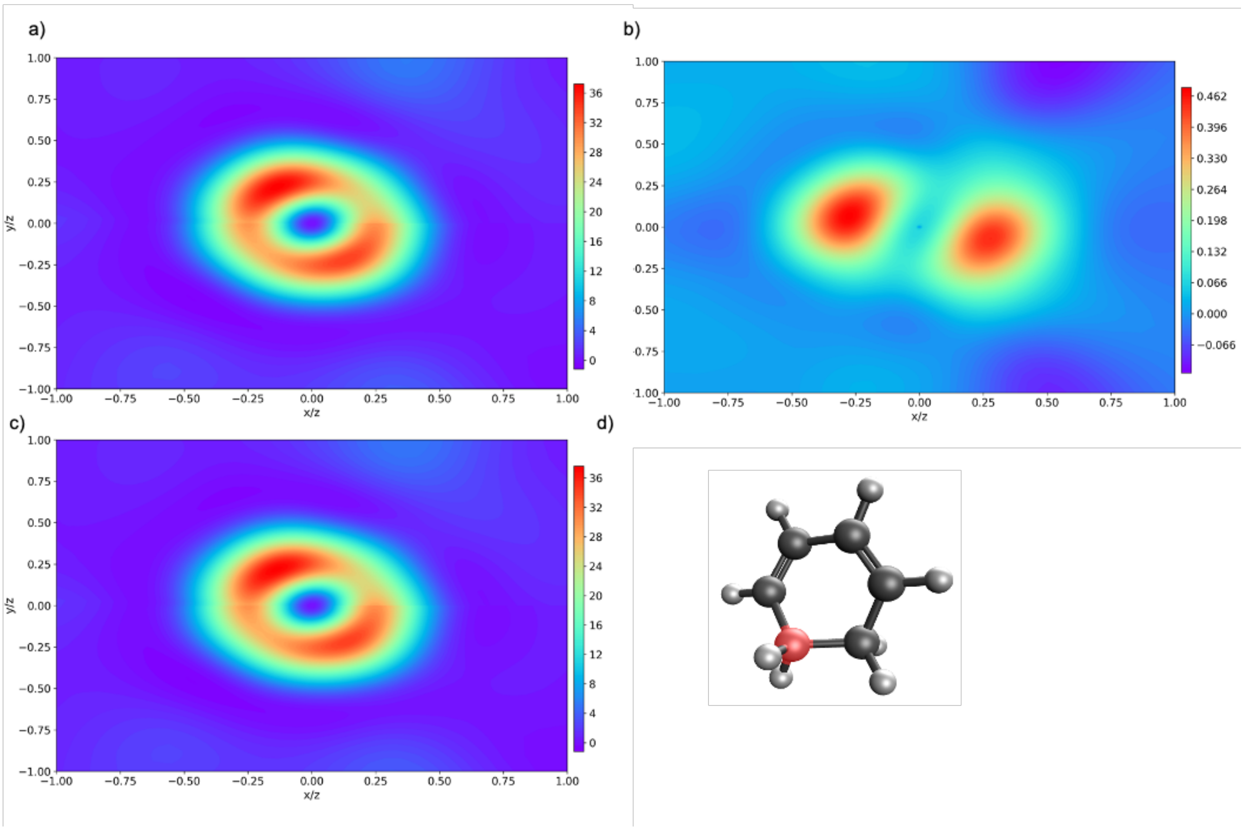

Figure S3: a) Difference between HF(6-311+G*) and IAM. b) The same as a) but using the cc-pCVQZ basis set in the HF calculation. c) Difference between HF(cc-pCVQZ) and HF(6-311+G*). d) Core hole state used throughout calculations. All calculations at 5.6 keV.

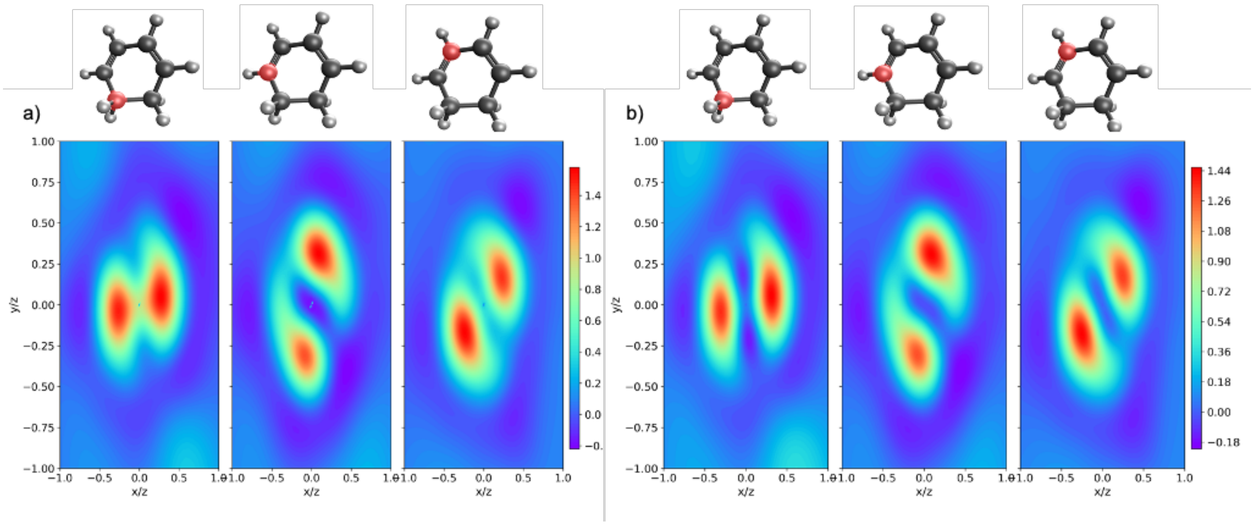

Figure S4: Difference between the DFT(6-311+G*) and HF(6-311+G*) coherent scattering cross sections at three core hole states at 5.6 keV. a) Numerical integration precision of 10^{-3} (used throughout the main text, b Numerical integration precision of 10^{-4}

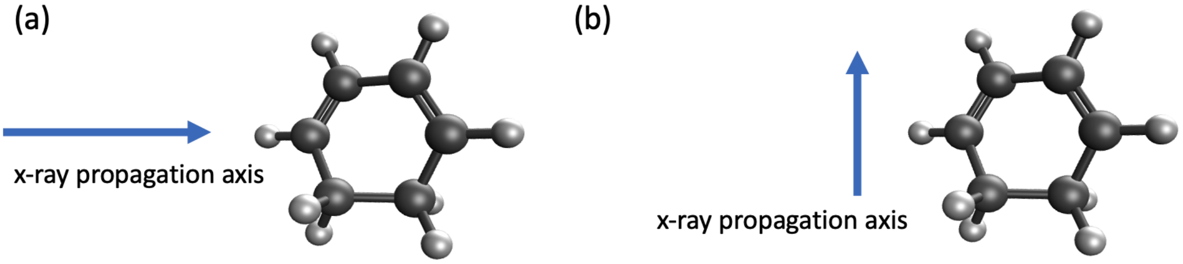

Figure S5: Two orientations of 1-3-cyclohexadiene with respect to the x-ray propagation axis.

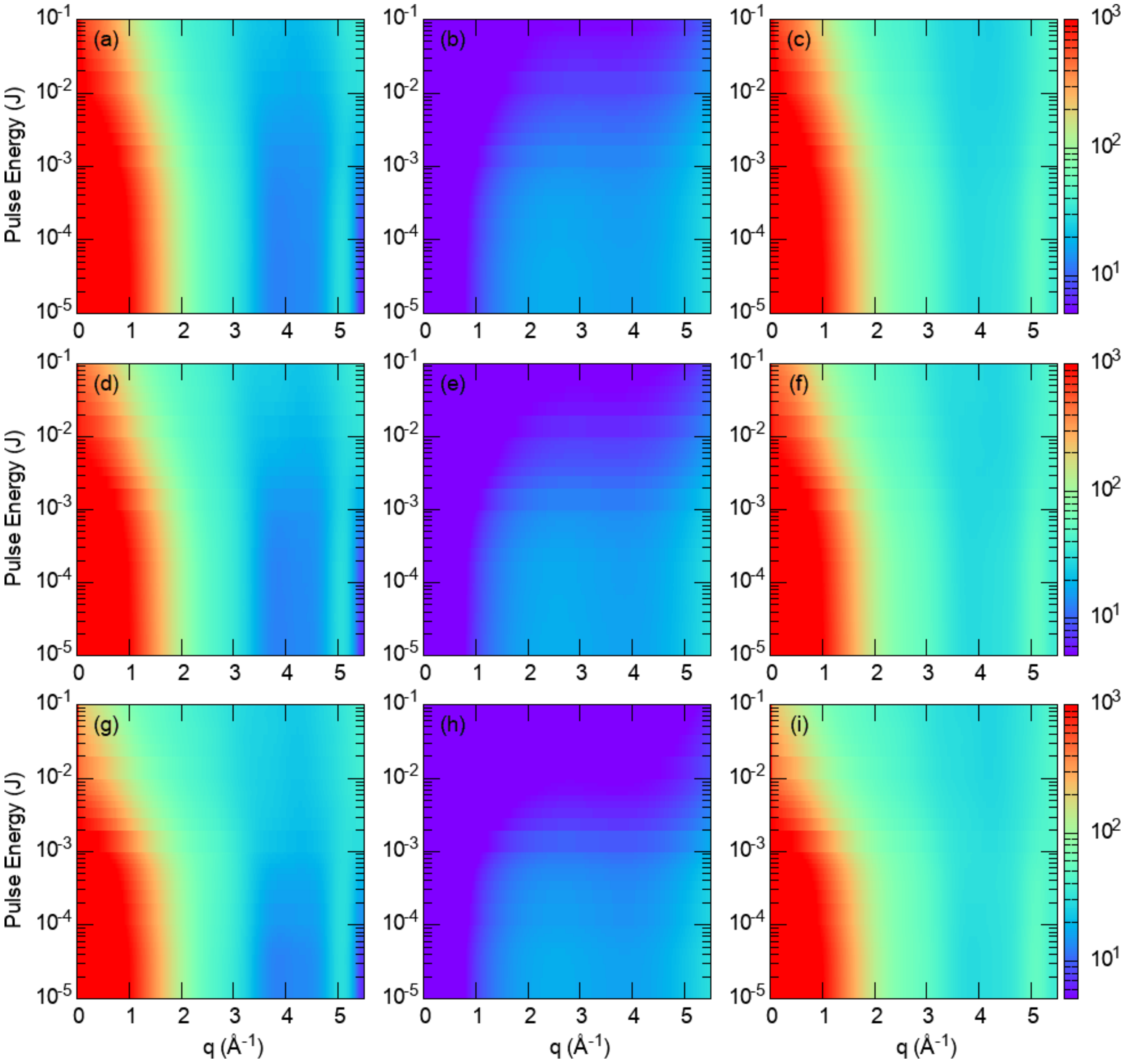

Figure S6: Pulse duration and pulse energy dependence of the azimuthally averaged differential x-ray scattering cross section of 1,3-cyclohexadiane exposed to an 5.6-keV pulse. Panel (a), (b) and (c) are the coherent, incoherent and the combined scattering cross sections calculated for a 0.25-fs pulse. Panel (d), (e) and (f) are for a 2.5-fs pulse, whereas panel (g), (h) and (i) are for a 25-fs pulse. The orientation of the molecule with respect to the x-ray is shown in Fig. S5 (a).

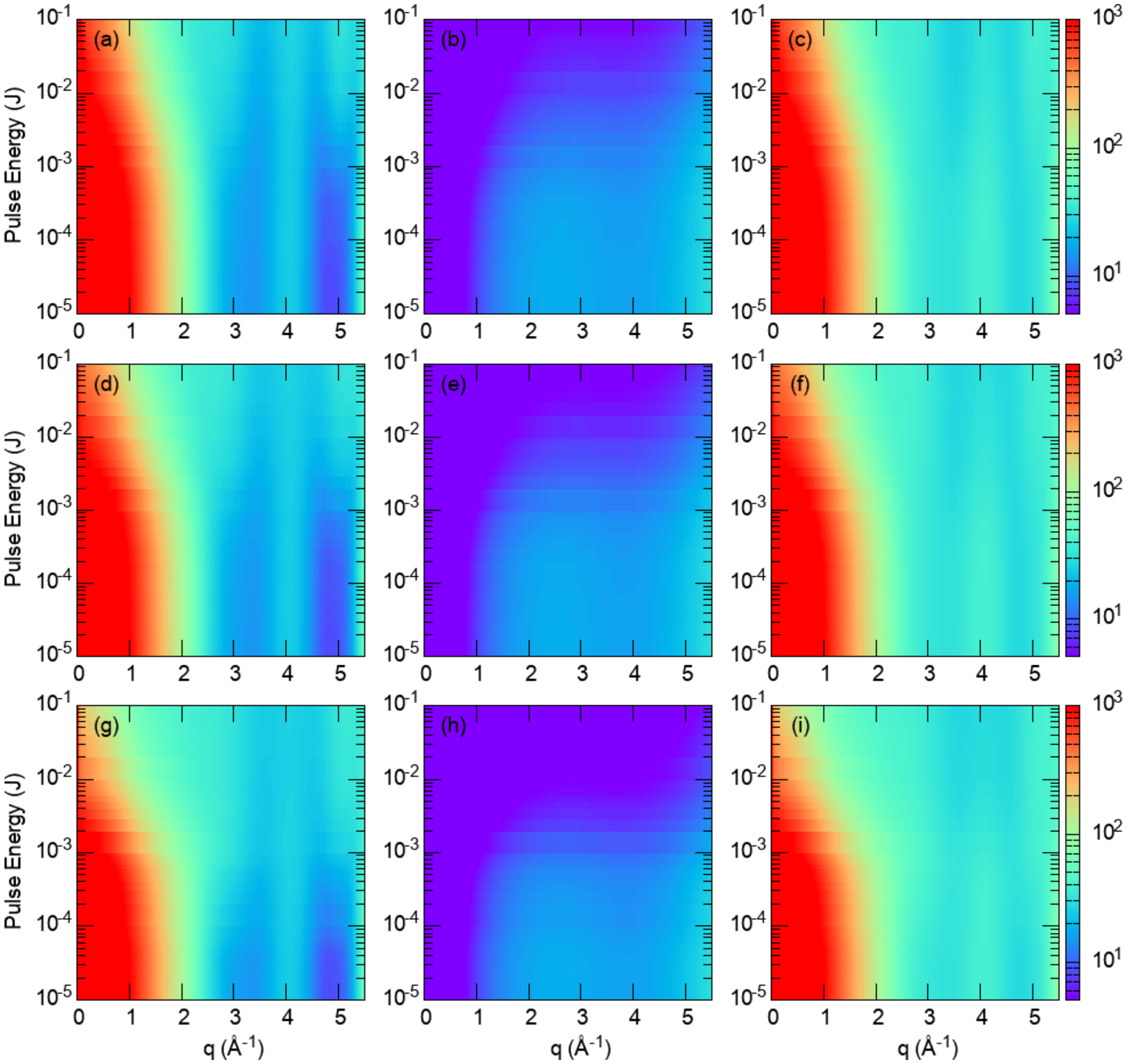

Figure S7: Same as Fig. S6, but the orientation of the molecule with respect to the x-ray is shown in Fig. S5 (b).

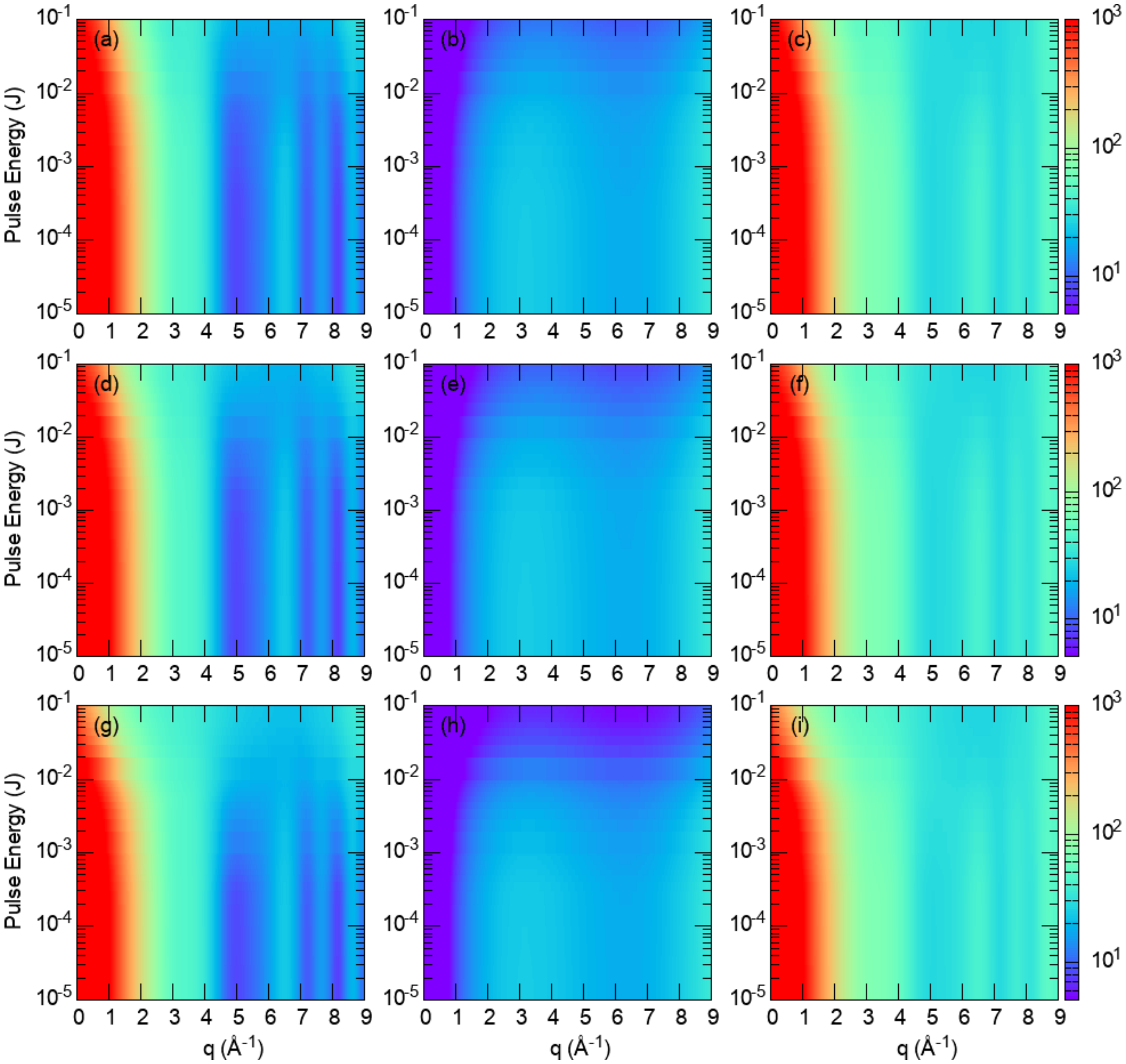

Figure S8: Same as Fig. S6, but the photon energy is 9 keV.

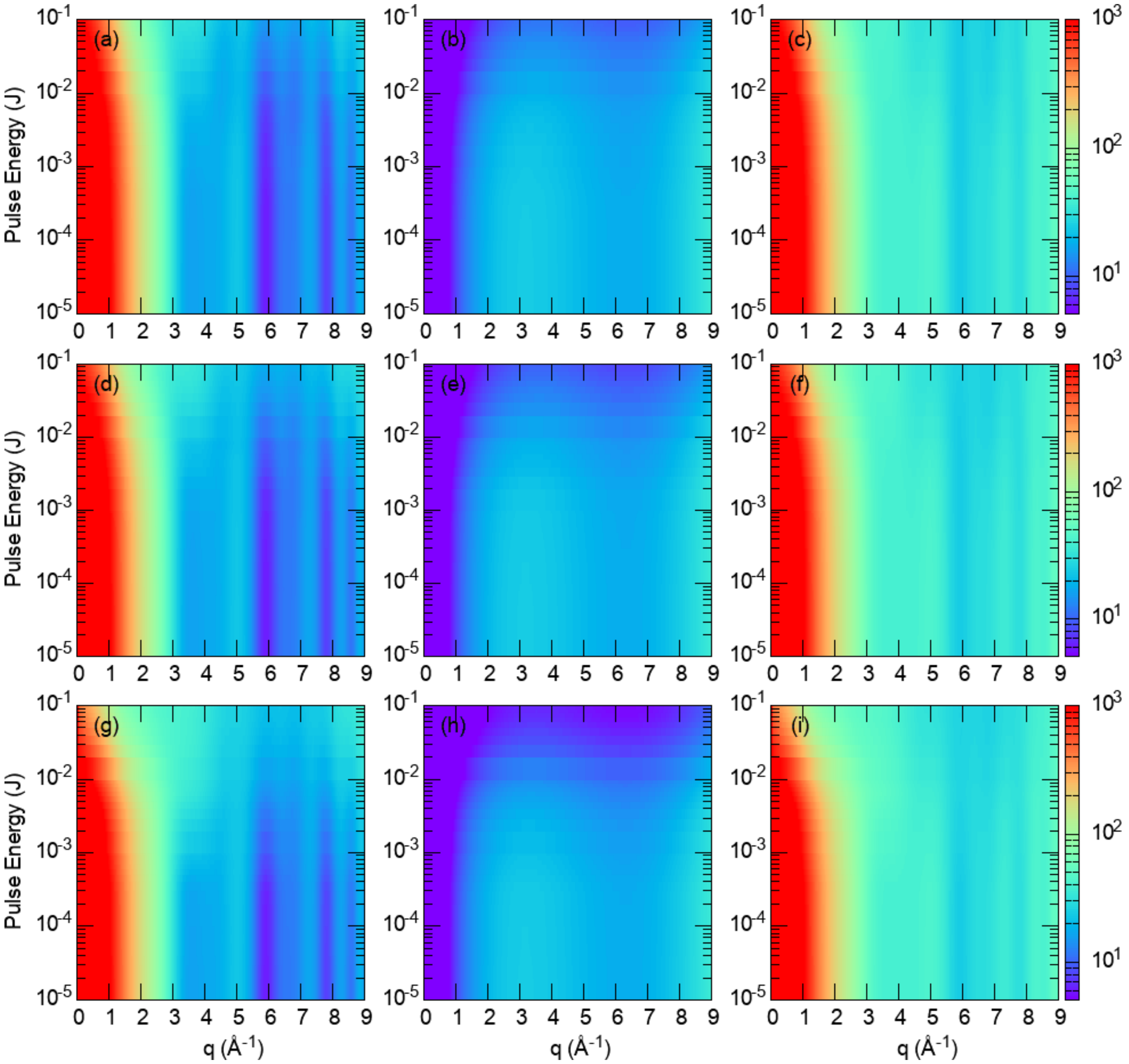

Figure S9: Same as Fig. S6, but the photon energy is 9 keV and the orientation of the molecule with respect to the x-ray is shown in Fig. S5 (b).

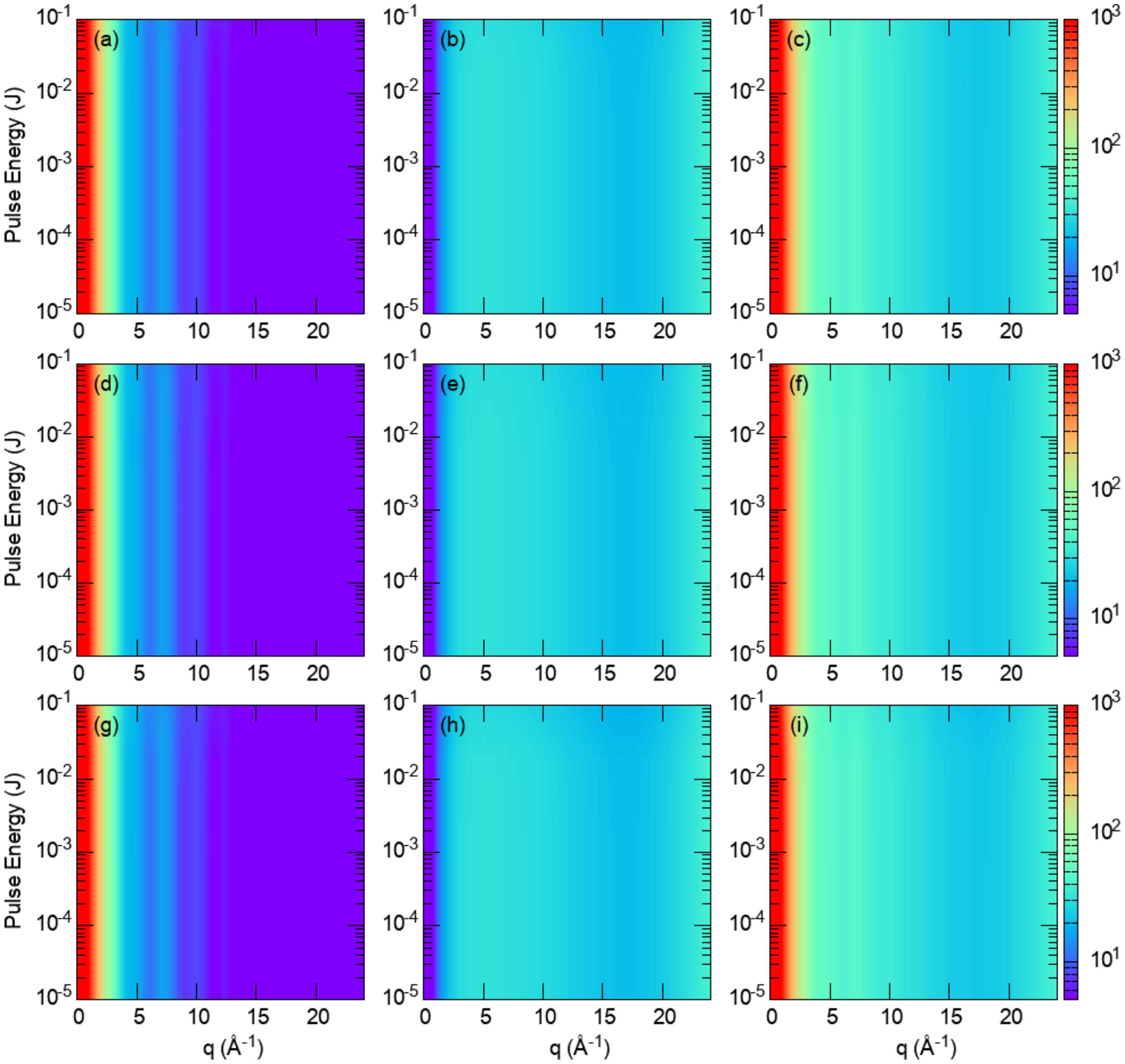

Figure S10: Same as Fig. S6, but the photon energy is 24 keV.

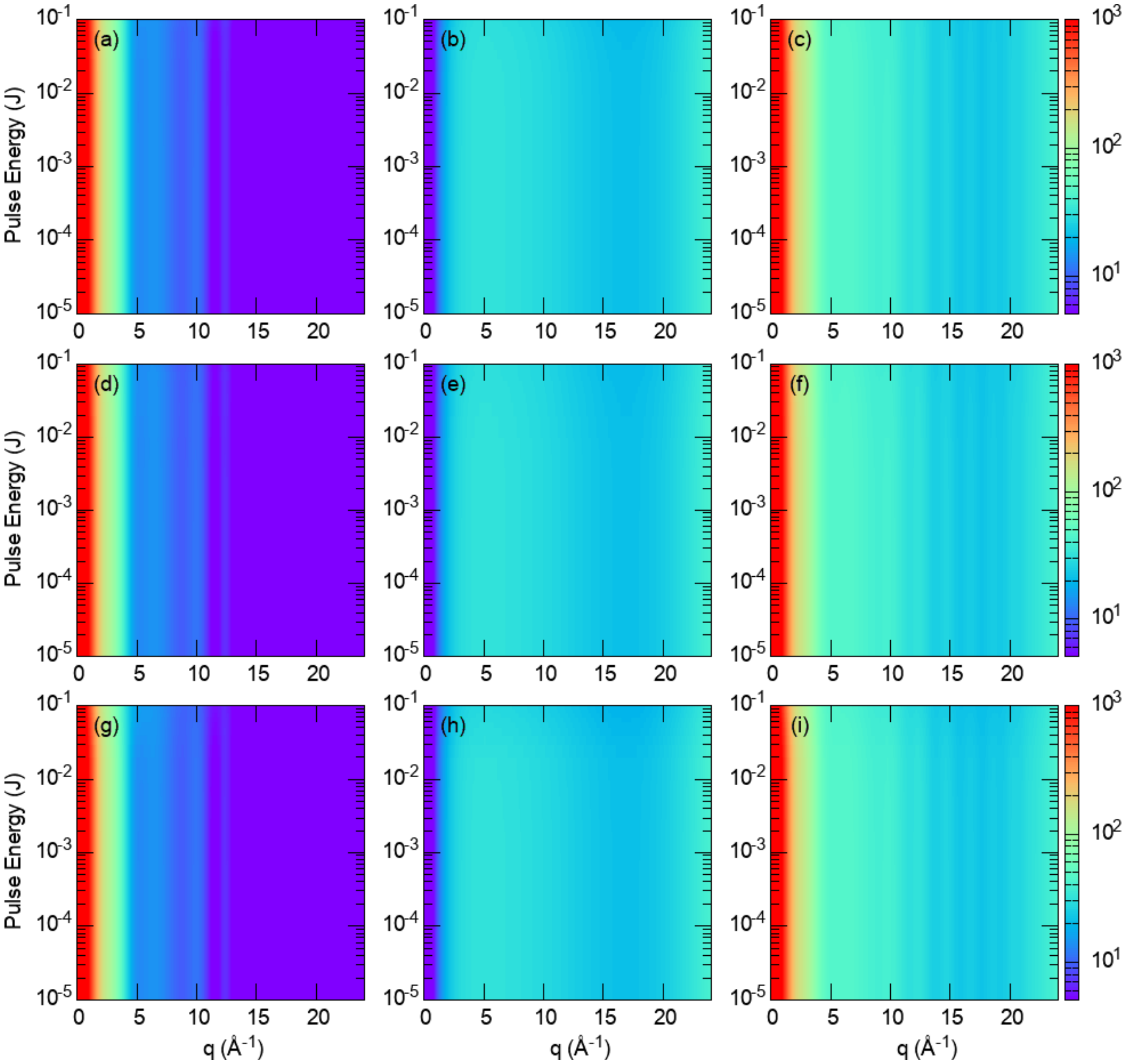

Figure S11: Same as Fig. S6, but the photon energy is 24 keV and the orientation of the molecule with respect to the x-ray is shown in Fig. S5 (b).