FOUNDATIONS
ADVANCES

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Supporting information for article:

Introduction of a weighting scheme for the X-ray restrained wavefunction approach: advantages and drawbacks

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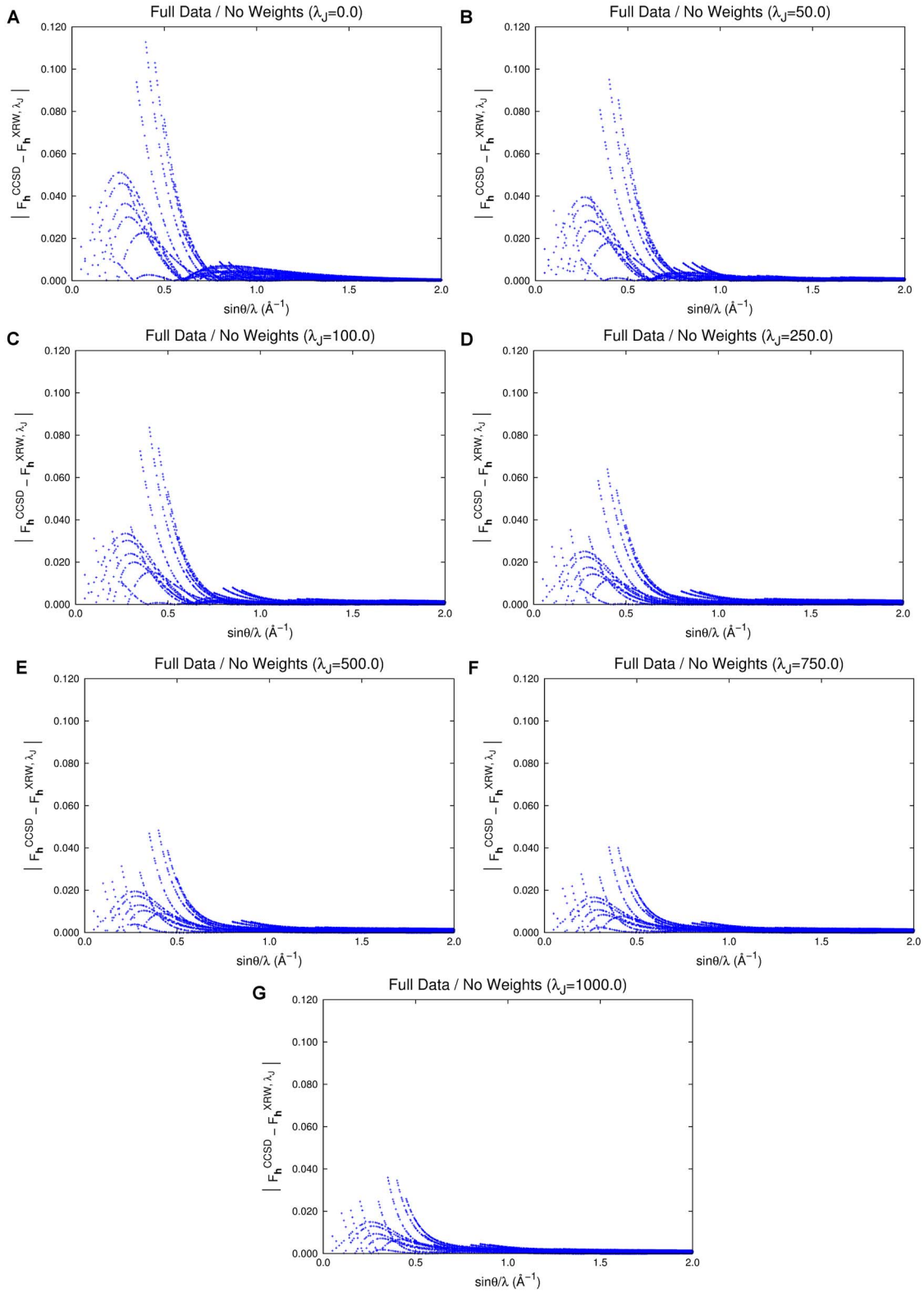

Figure S1 Absolute differences between calculated and reference structure factor amplitudes at different values of λ_J for the XRW calculation performed without applying the proposed weighting scheme and by exploiting the full set of X-ray diffraction data corresponding to the gas-phase CCSD/UGBS electron density of HCN.

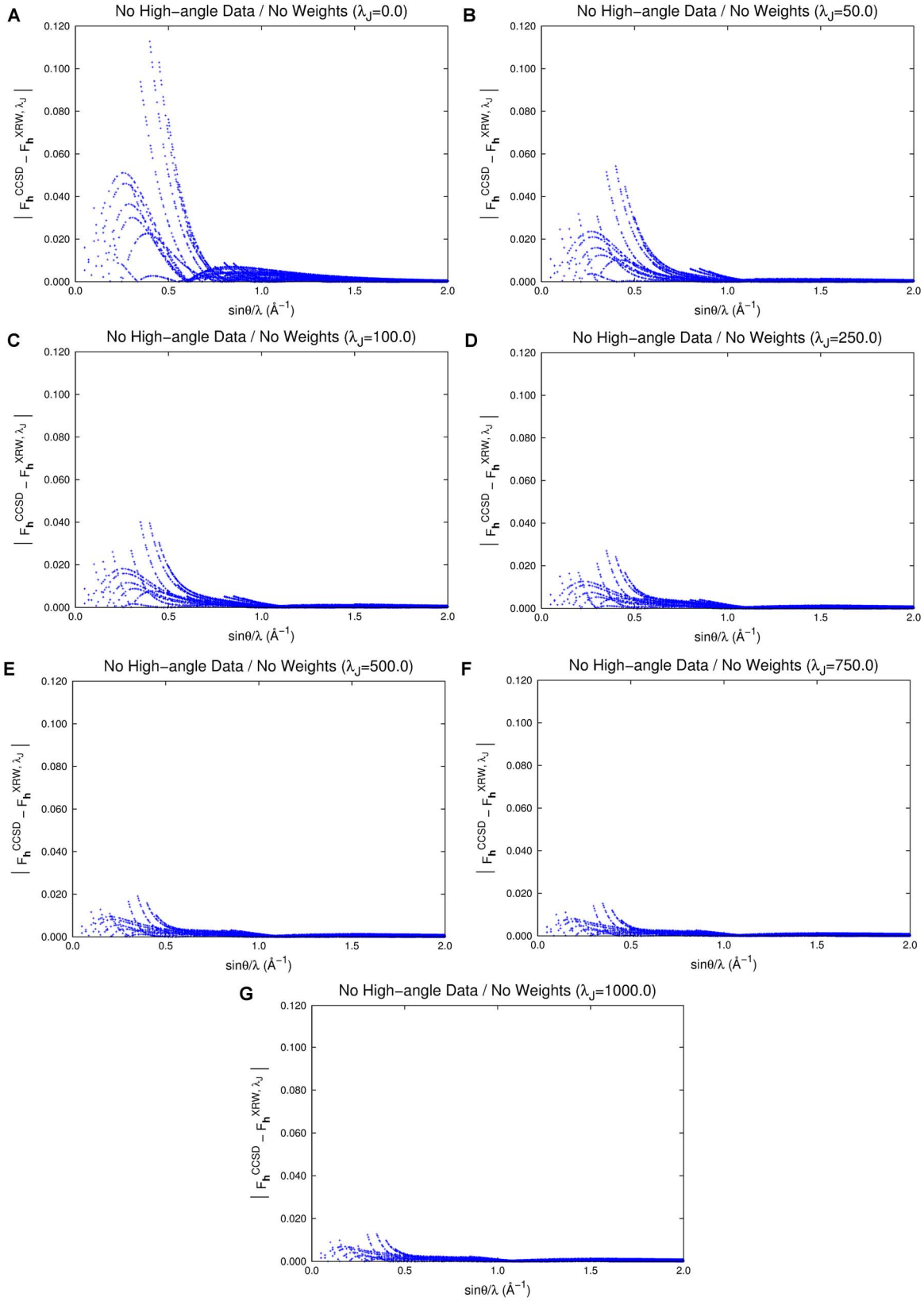

Figure S2 Absolute differences between calculated and reference structure factor amplitudes at different values of λ_J for the XRW calculation performed without applying the proposed weighting

scheme and by exploiting only the low- and medium-angle sets of X-ray diffraction data corresponding to the gas-phase CCSD/UGBS electron density of HCN.

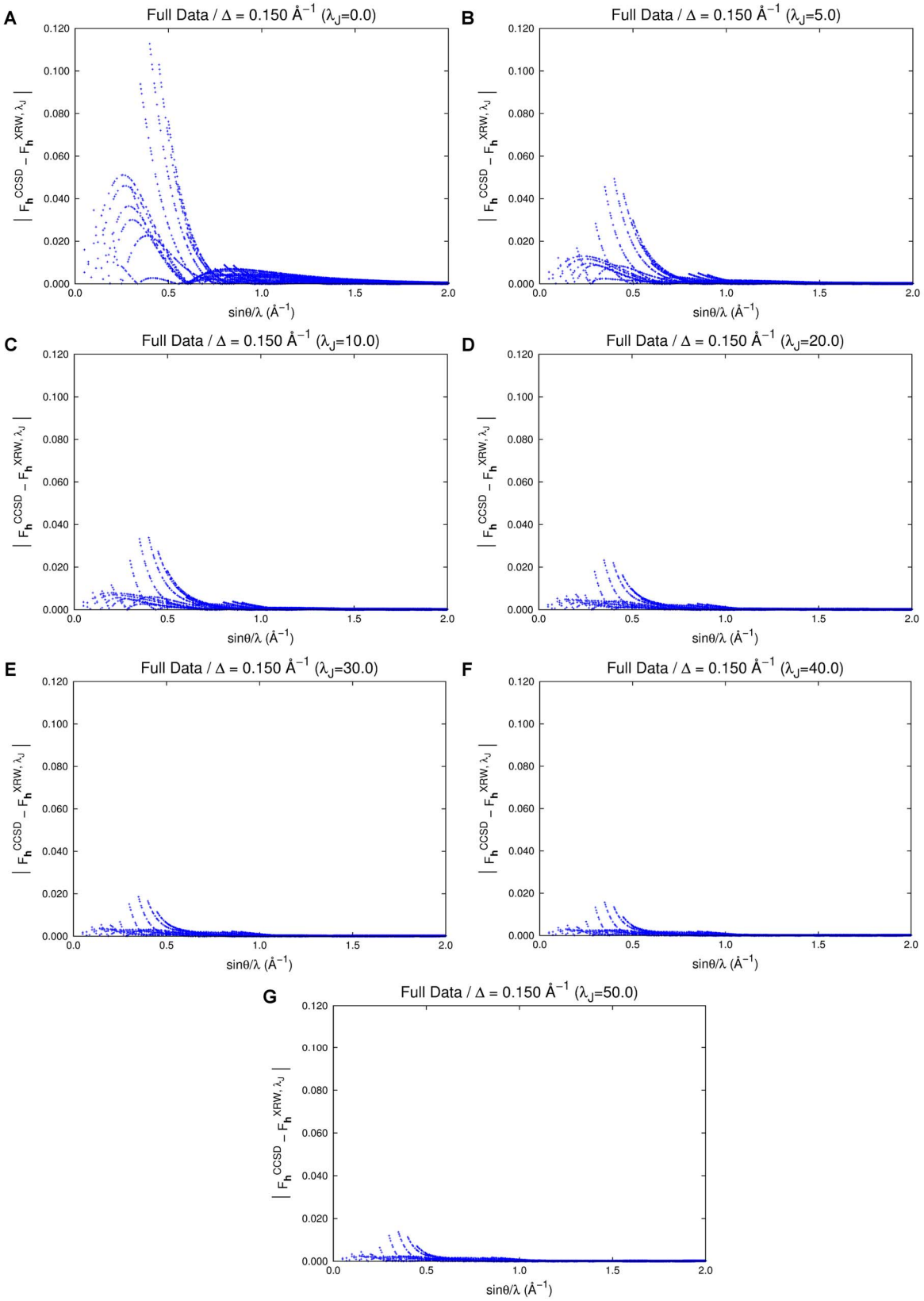

Figure S3 Absolute differences between calculated and reference structure factor amplitudes at different values of λ_J for the XRW calculation performed by applying the proposed weighting scheme

($\Delta = 0.150$ Å^{-1}) and by exploiting the full set of X-ray diffraction data corresponding to the gas-phase CCSD/UGBS electron density of HCN.

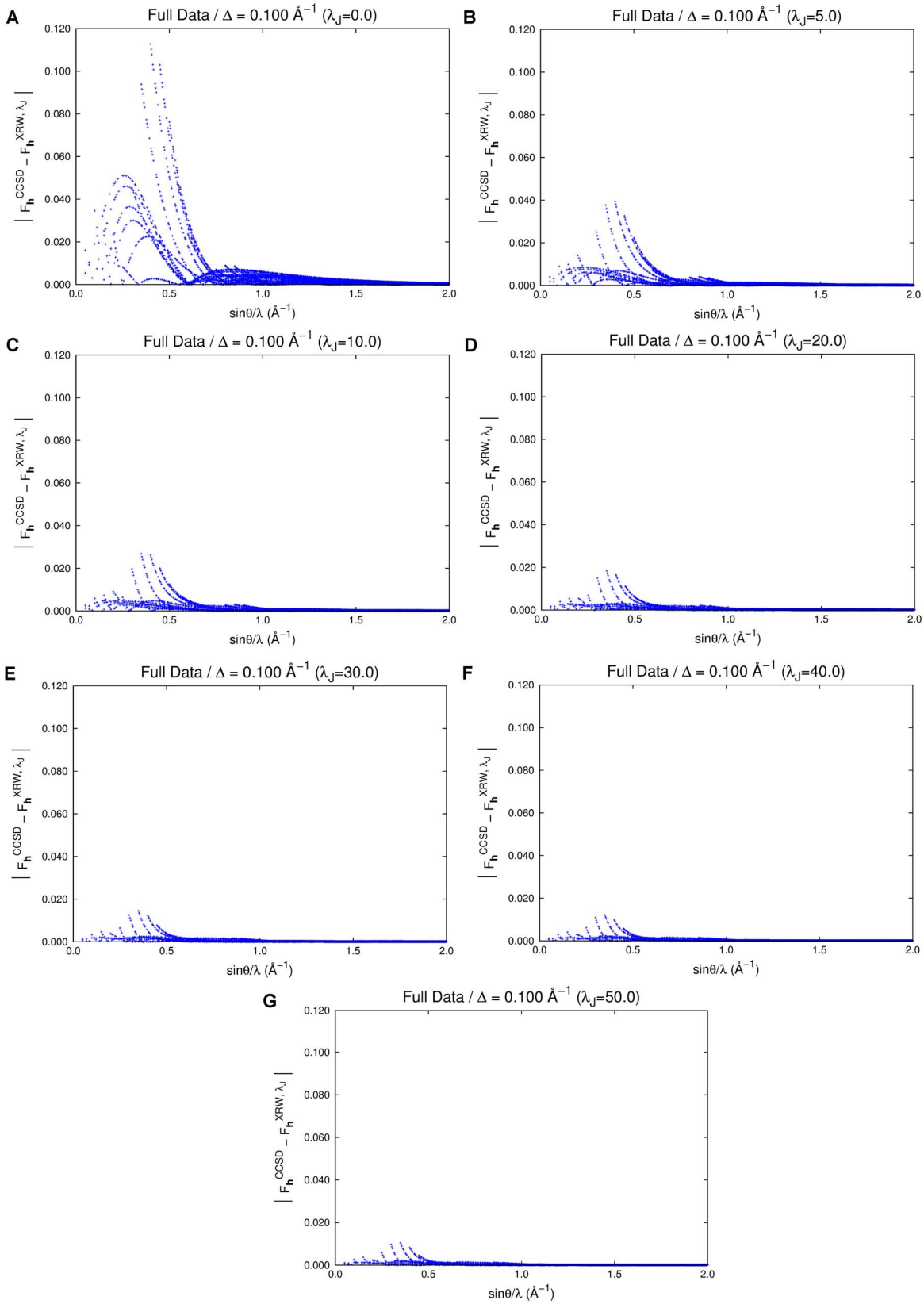

Figure S4 Absolute differences between calculated and reference structure factor amplitudes at different values of λ_J for the XRW calculation performed by applying the proposed weighting scheme

($\Delta = 0.100$ Å^{-1}) and by exploiting the full set of X-ray diffraction data corresponding to the gas-phase CCSD/UGBS electron density of HCN.

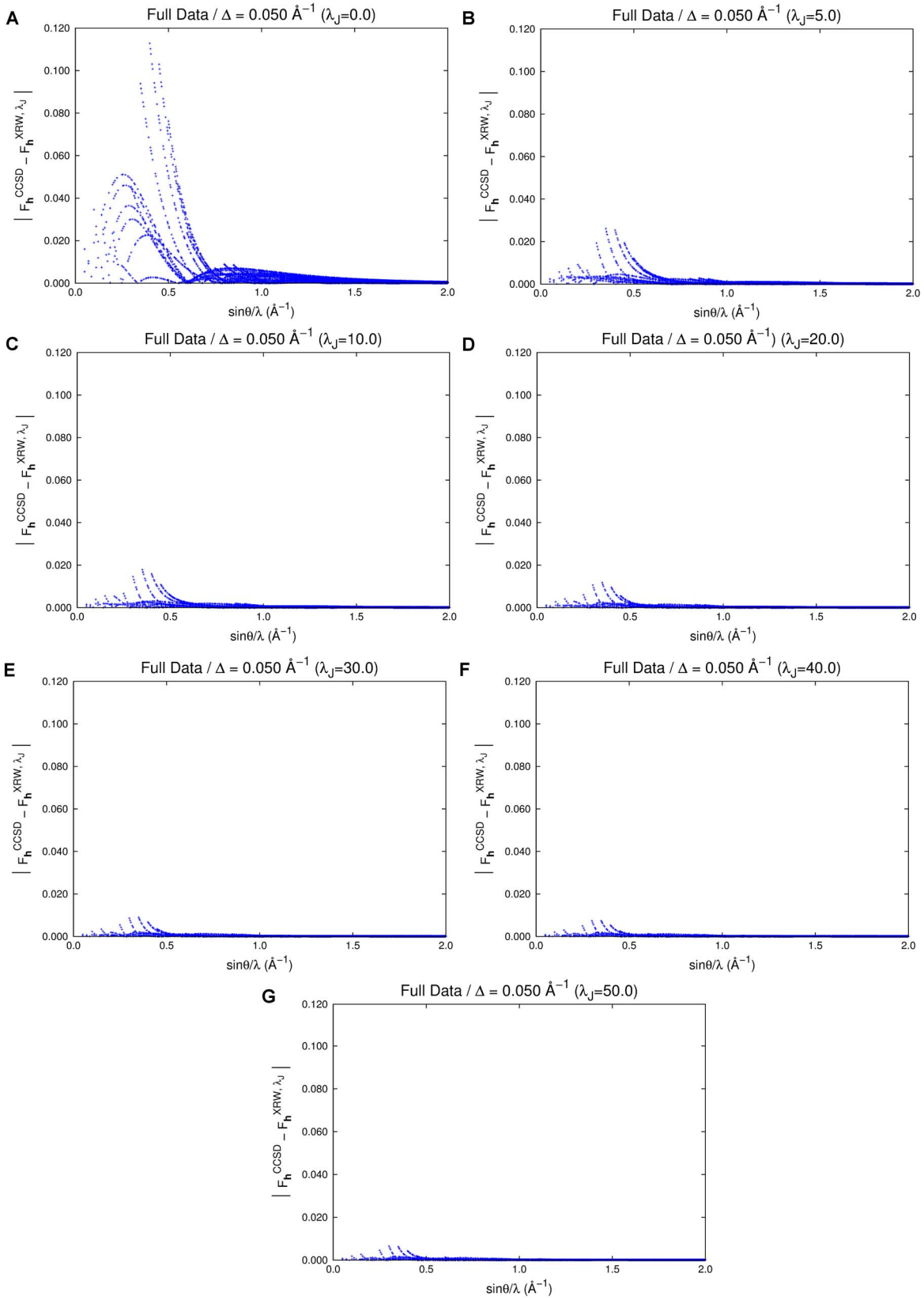

Figure S5 Absolute differences between calculated and reference structure factor amplitudes at different values of λ_J for the XRW calculation performed by applying the proposed weighting scheme

($\Delta = 0.050$ Å^{-1}) and by exploiting the full set of X-ray diffraction data corresponding to the gas-phase CCSD/UGBS electron density of HCN.

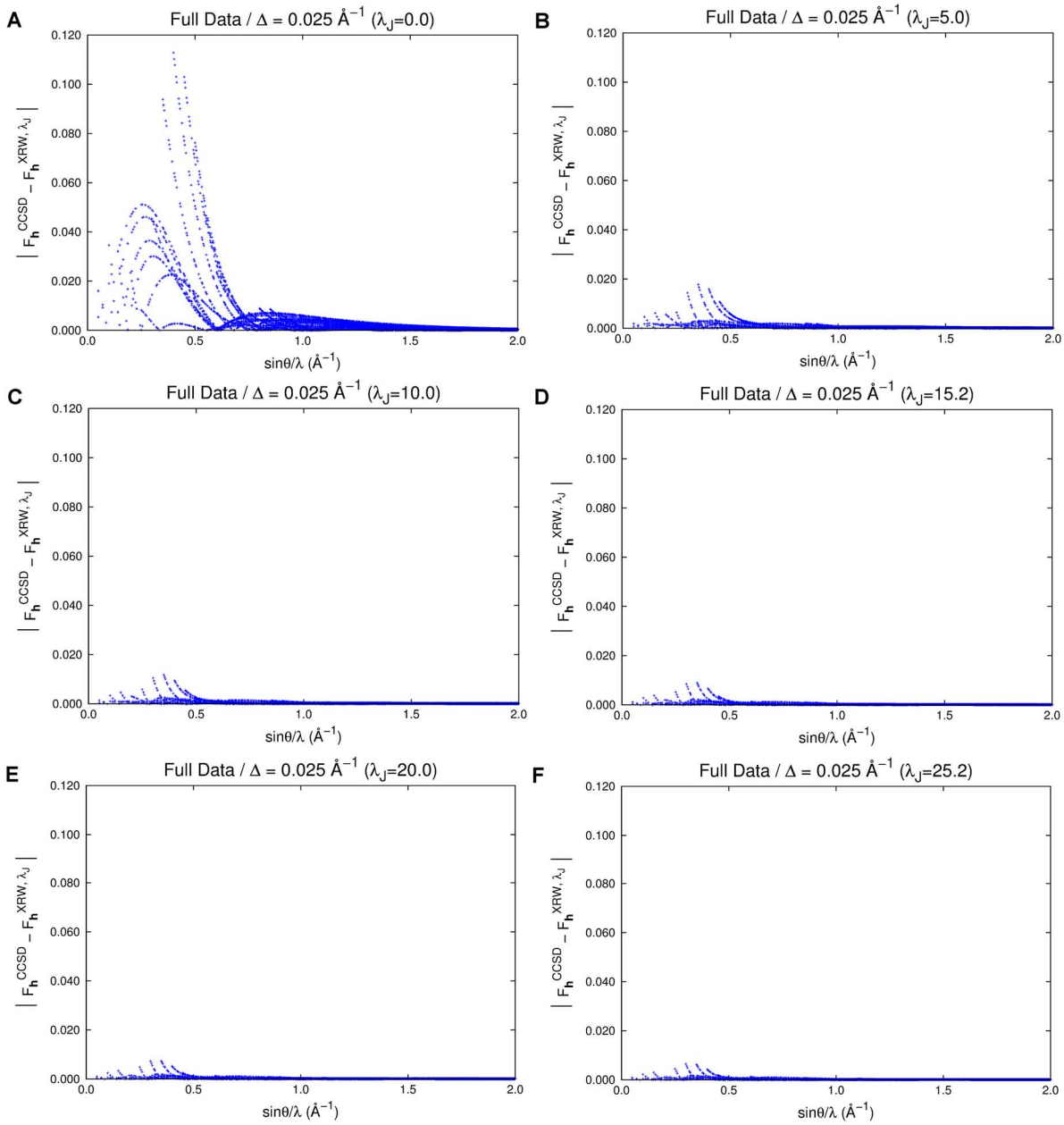

Figure S6 Absolute differences between calculated and reference structure factor amplitudes at different values of λ_J for the XRW calculation performed by applying the proposed weighting scheme ($\Delta = 0.025$ Å^{-1}) and by exploiting the full set of X-ray diffraction data corresponding to the gas-phase CCSD/UGBS electron density of HCN.

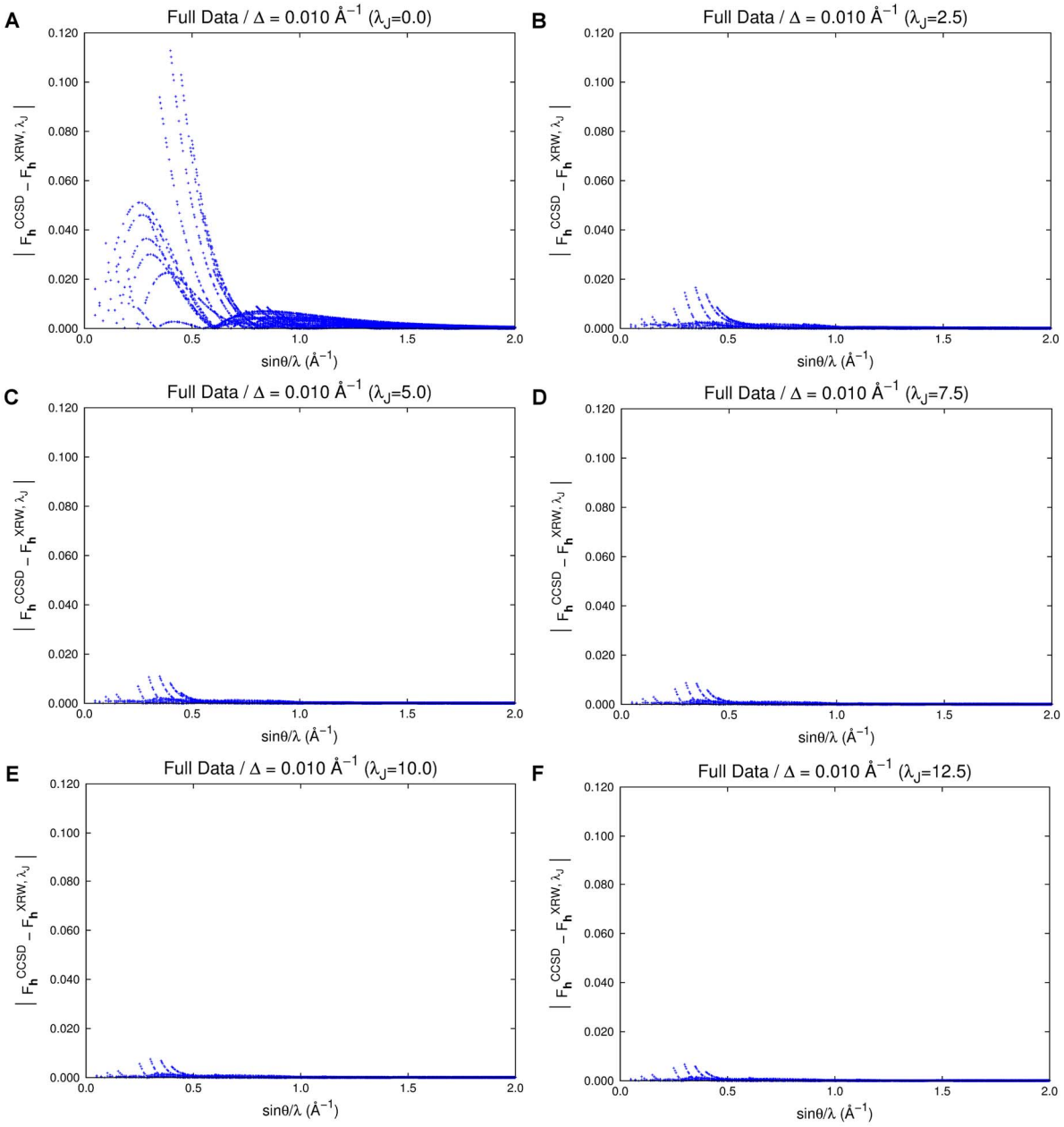

Figure S7 Absolute differences between calculated and reference structure factor amplitudes at different values of λ_J for the XRW calculation performed by applying the proposed weighting scheme ($\Delta = 0.010$ Å^{-1}) and by exploiting the full set of X-ray diffraction data corresponding to the gas-phase CCSD/UGBS electron density of HCN.

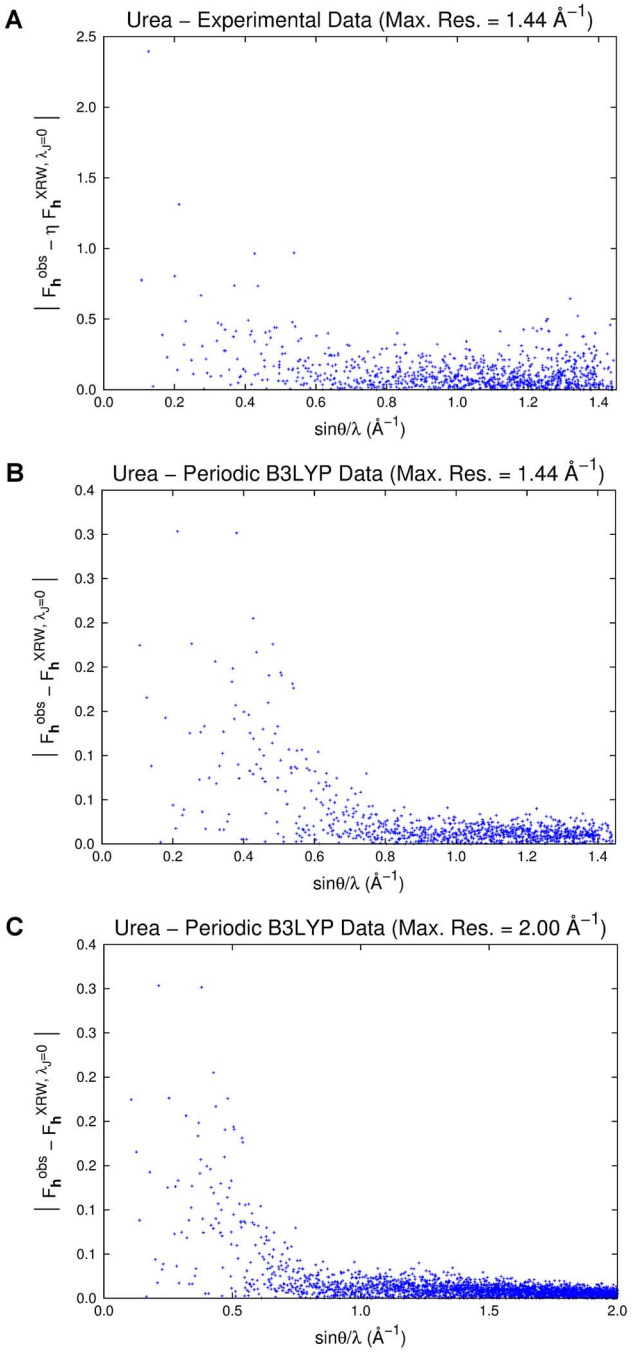

Figure S8 Absolute differences between reference and unrestrained ($\lambda_J = 0$) structure factor amplitudes in the case of (A) experimental X-ray diffraction data for urea, (B) X-ray diffraction data corresponding to the periodic B3LYP/cc-pVTZ electron density of urea ($(sin\theta/\lambda)_{max} = 1.44$ Å^{-1}), and (C) X-ray diffraction data corresponding to the periodic B3LYP/cc-pVTZ electron density of urea ($(sin\theta/\lambda)_{max} = 2.00$ Å^{-1}).