Fig. 5-1. The ratio patterns from diffraction by (a) chlorobenzene and (b) bromobenzene.
Fig. 5-2. The final refined theory (line) with experimental data (filled squares) for chlorobenzene in (a) $sM(s)$ and (b) $f(r)$ representations. The fitted theory is quantified with $\chi^2 = 233.021$ and $R = 0.110$. The vertical bars at each peak position have a height proportional to $nZZ/r$. 
Fig. 5-3. $sM(s)$ curves for bromobenzene showing theory (line) with experimental data (filled squares). The theoretical curve in (a) corresponds to that derived from the DFT structure ($\chi^2 = 1137.568; \ R = 0.241$) and that in (b) is the DFT structure with a refined C–Br bond distance ($\chi^2 = 201.465; \ R = 0.104$).
Fig. 5-4. The final refined theory (line) with experimental data (filled squares) for bromobenzene in (a) $sM(s)$ and (b) $f(r)$ representations. The fitted theory is quantified with $\chi^2 = 70.166$ and $R = 0.061$. The vertical bars at each peak position have a height proportional to $nZ_iZ_j/r$. 
Fig. 5-5. The ratio patterns from diffraction by (a) iodobenzene and (b) 2-fluoropyridine.
Fig. 5-6. $sM(s)$ curves for iodobenzene showing theory (line) with experimental data (filled squares). The theoretical curve in (a) corresponds to that derived from the DFT structure ($\chi^2 = 259.793; R = 0.173$) and that in (b) is the DFT structure with a refined C-I bond distance ($\chi^2 = 88.392; R = 0.102$).
Fig. 5-7. The final refined theory (line) with experimental data (filled squares) for iodobenzene in (a) $sM(s)$ and (b) $f(r)$ representations. The fitted theory is quantified with $\chi^2 = 69.192$ and $R = 0.089$. The vertical bars at each peak position have a height proportional to $nZ_iZ_j/r$. 
Fig. 5-8. The final refined theory (line) with experimental data (filled squares) for 2-fluoropyridine in (a) $sM(s)$ and (b) $f(r)$ representations. The fitted theory is quantified with $\chi^2 = 89.686$ and $R = 0.035$. 
Fig. 5-9. The ratio patterns from diffraction by (a) acetylacetone and (b) benzaldehyde.
Fig. 5-10. The final refined theory (line) with experimental data (filled squares) for acetylacetone in (a) $sM(s)$ and (b) $f(r)$ representations. The fitted theory is quantified with $\chi^2 = 41.676$ and $R = 0.030$. The $f(r)$ is broken up to show individual contribution from both enol (dashed) and keto (dotted) tautomers.
Fig. 5-11. $sM(s)$ curves for various models with refined component fractional contributions. (a) 86% DFT C, enol + 14% DFT keto tautomer; $\chi^2 = 198.320$; $R = 0.066$. (b) 67% DFT C, enol + 33% DFT keto tautomer; $\chi^2 = 1423.836$; $R = 0.174$. (c) 78% refined C, enol + 22% refined keto tautomer; $\chi^2 = 41.676$; $R = 0.030$. The solid line below each plot is the residual (theory – experiment).
Fig. 5-12. The final refined theory (line) with experimental data (filled squares) for benzaldehyde in (a) $sM(s)$ and (b) $f(r)$ representations. The fitted theory is quantified with $\chi^2 = 67.127$ and $R = 0.043$. 
Fig. 5-13. The ratio patterns from diffraction by (a) acetophenone and (b) methylbenzoate.
Fig. 5-14. The final refined theory (line) with experimental data (filled squares) for acetophenone in (a) $sM(s)$ and (b) $f(r)$ representations. The fitted theory is quantified with $\chi^2 = 39.069$ and $R = 0.028$. 
Fig. 5-15. The final refined theory (line) with experimental data (filled squares) for methylbenzoate in (a) $sM(s)$ and (b) $f(r)$ representations. The fitted theory is quantified with $\chi^2 = 224.746$ and an $R = 0.056$. 

Chapter 5. Ground-state Molecular Structure