

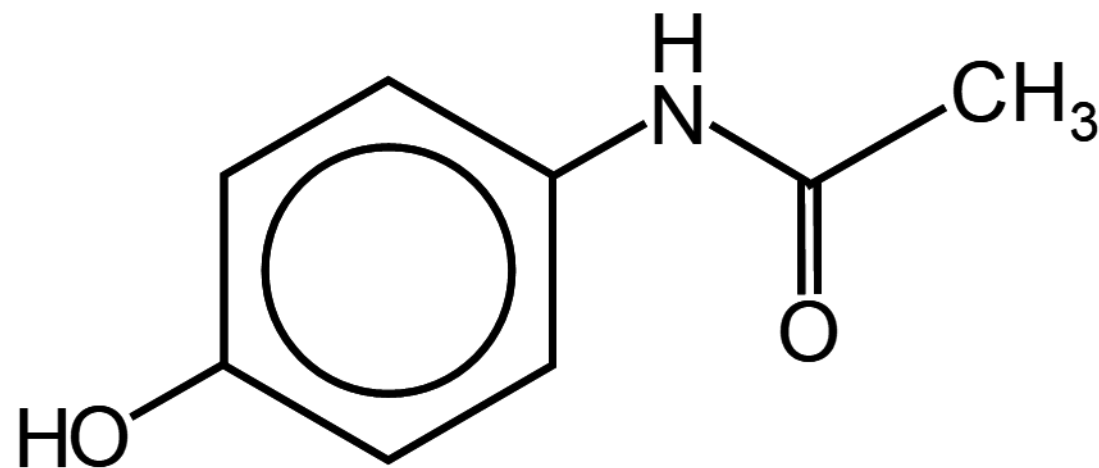
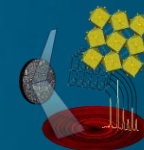


Figure 25.1. Illustration of the molecular structure of acetaminophen, $C_8H_9NO_2$. The carbon and hydrogen atoms in the phenyl ring are not labeled for clarity.

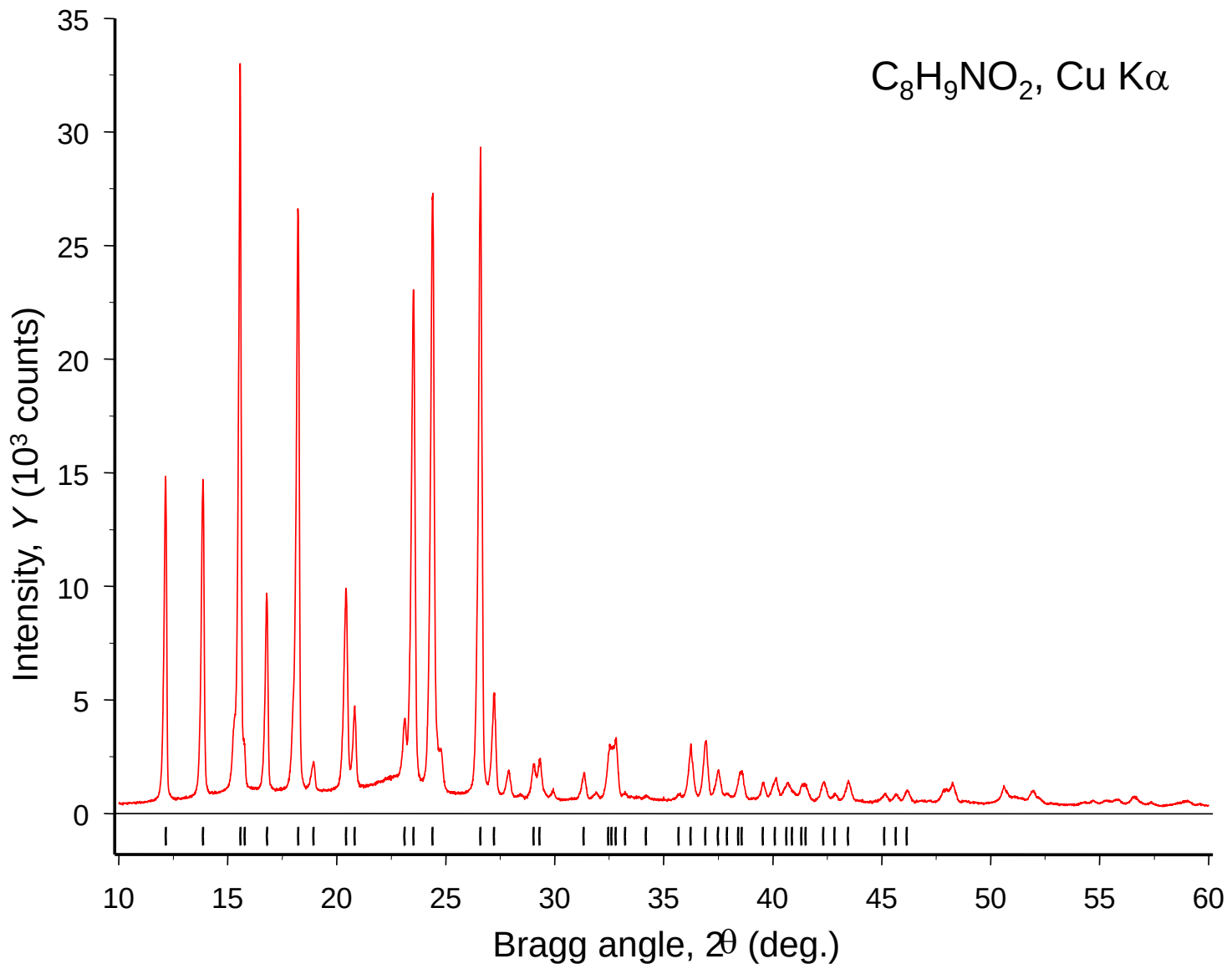
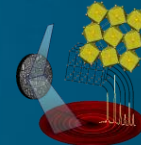


Figure 25.2. Powder diffraction pattern collected from two ground Tylenol[®] pills using Cu $K\alpha$ radiation on a Bruker D8 Advance diffractometer equipped with SolX detector. The vertical bars indicate positions of the $K\alpha_1$ components of the Bragg peaks observed below $47^\circ 2\theta$.

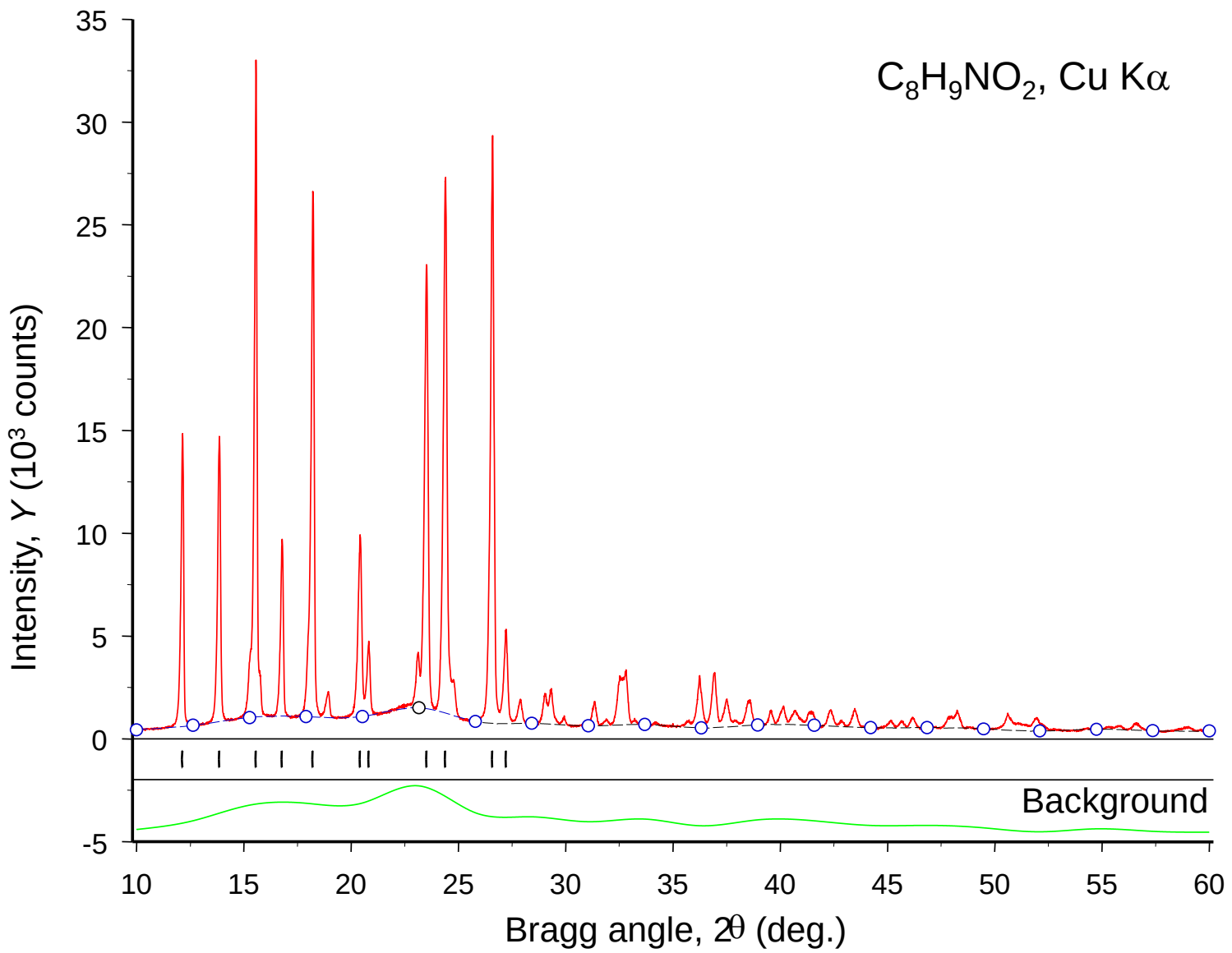
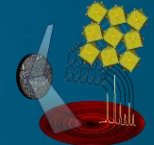


Figure 25.3. Experimental powder diffraction pattern of acetaminophen (*red solid line*) and the background (*blue dashed line*) determined automatically using the 20-point Bayesian spline interpolation. The *green solid line* at the *bottom* shows the background enlarged by a factor of two along the intensity axis revealing the presence of amorphous phases. The *vertical bars* indicate positions of the Kα₁ components of the Bragg peaks found by the automatic peak search routine.

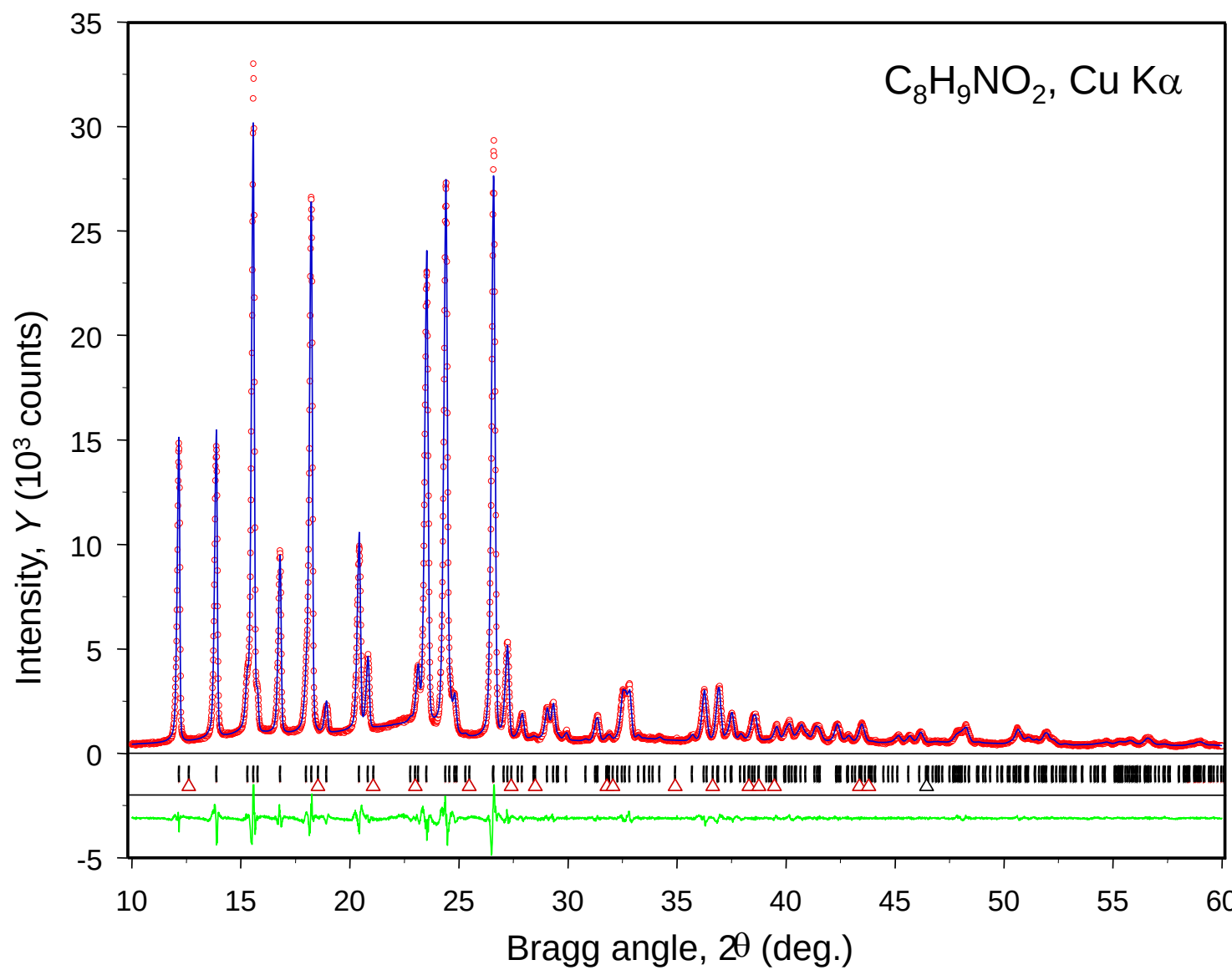
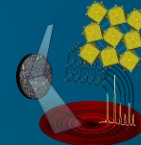


Figure 25.4. Le Bail fit showing the observed (red circles) and calculated (blue solid line) diffraction patterns of acetaminophen. The vertical bars indicate calculated positions of the $K\alpha_1$ components of Bragg peaks. The open red triangles indicate locations of reflections that are forbidden in the space group $P2_1/n$. The green solid line at the bottom represents the difference between the observed and calculated profiles.

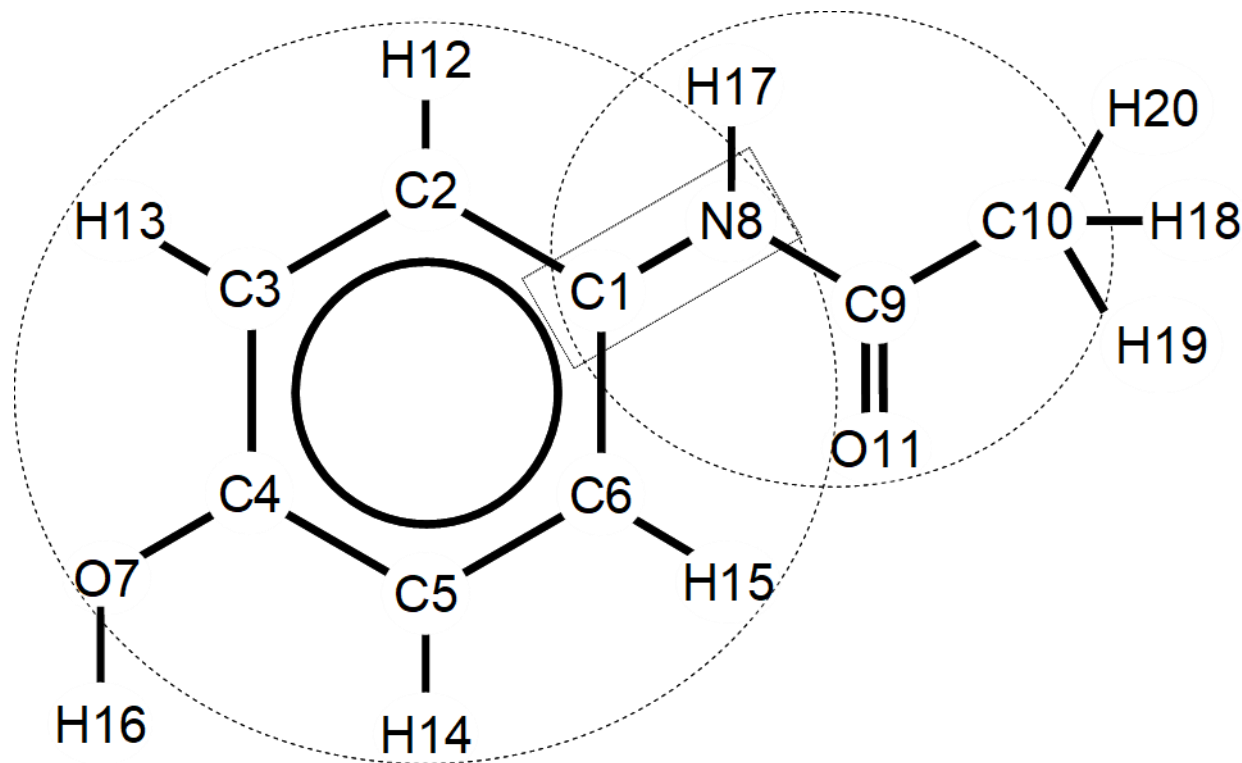
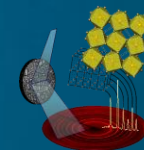


Figure 25.5. The numerical scheme identifying all atoms in the molecule of acetaminophen. The *dashed ellipses* encircle two flat rigid groups and the solid rectangle encloses a common bond around which the rigid groups may rotate relatively to one another.

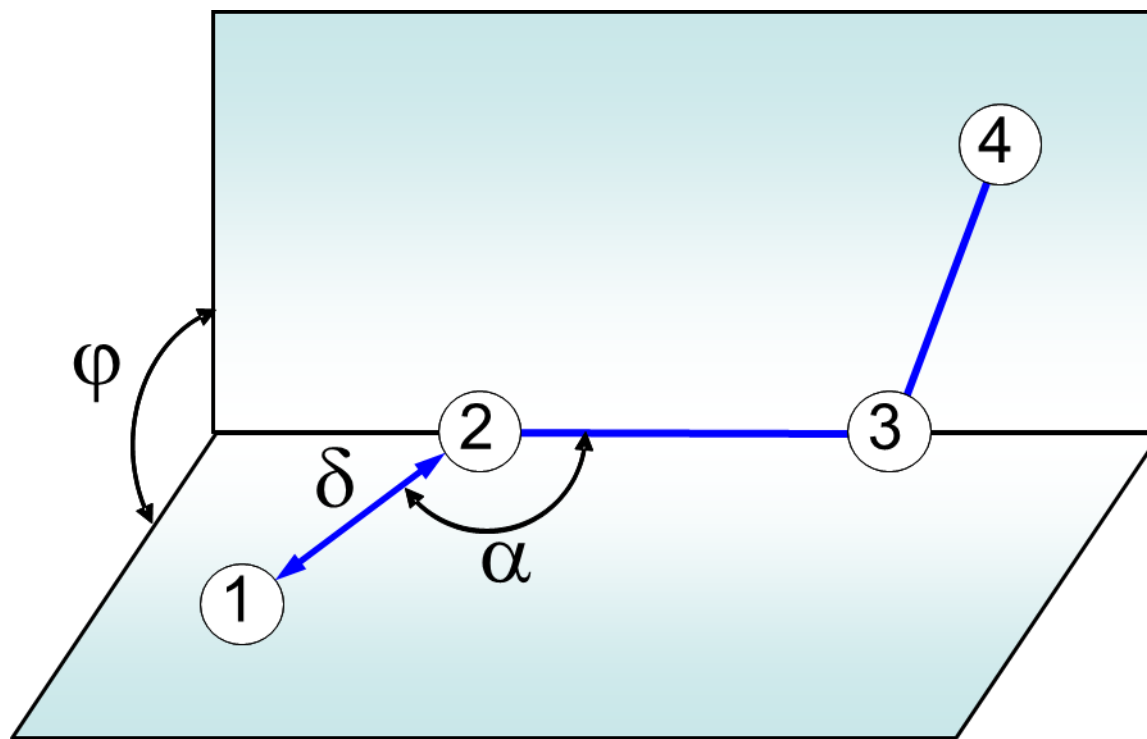
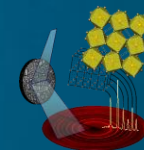


Figure 25.6. Illustration of how to derive the location of a new atom (atom 1) from the triplet of known atoms (atoms 2, 3, and 4) by specifying the distance between atoms 1 and 2 (δ_{12}), the angle α_{123} and the torsion angle φ_{1234} . The torsion or dihedral angle describes the conformation of four atoms 1, 2, 3, and 4, and it is defined as the angle between the two planes formed by atoms 1, 2, 3, and 2, 3, and 4, respectively.

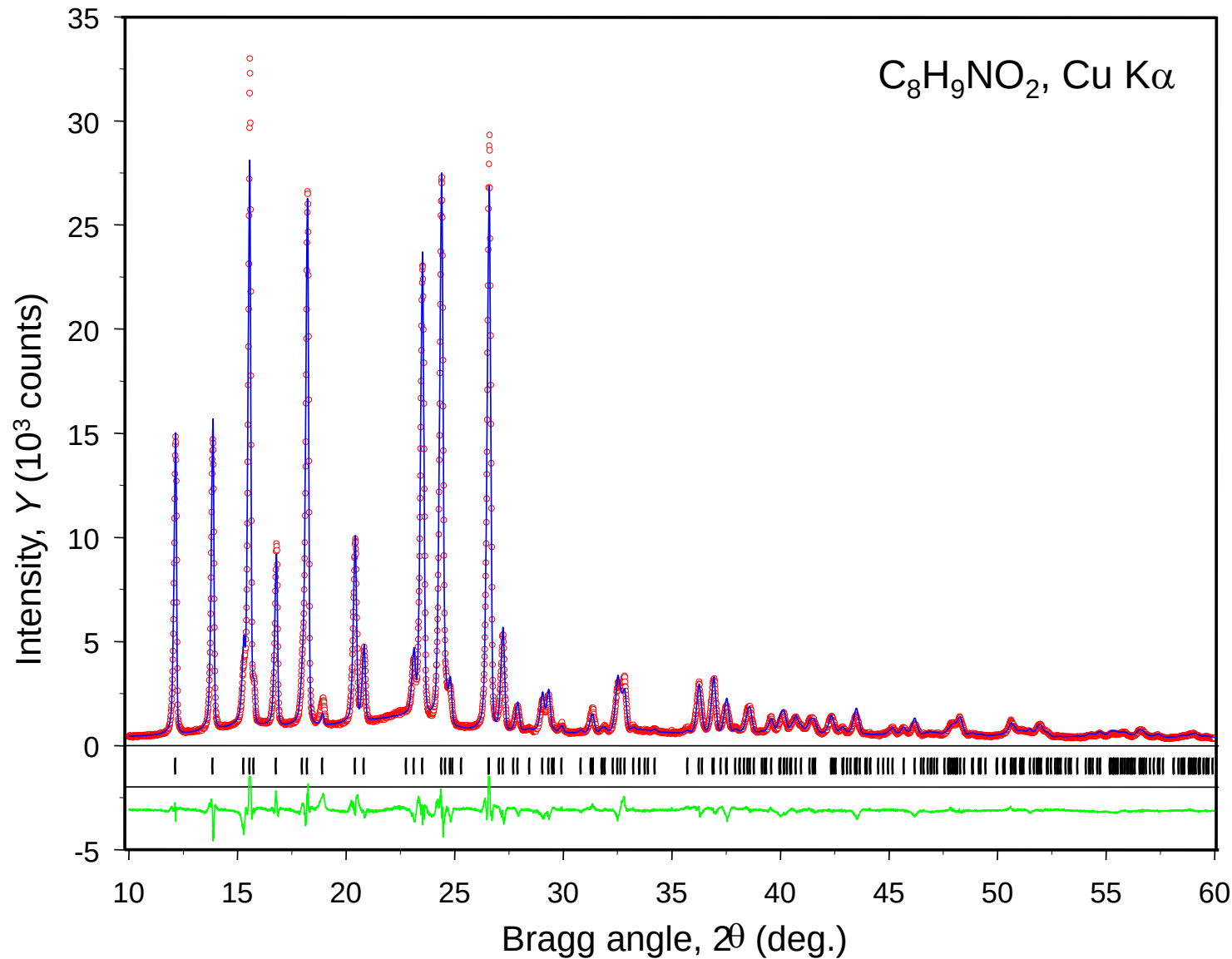
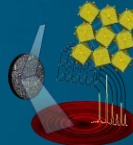


Figure 25.7. Result of solving the acetaminophen structure using FOX parallel tempering optimization, showing the observed (*red circles*) and calculated (*blue solid line*) diffraction patterns. The *vertical bars* indicate the positions of the $K\alpha_1$ components of calculated reflections. The oscillating curve at the *bottom* shows the difference between the observed and calculated profiles.

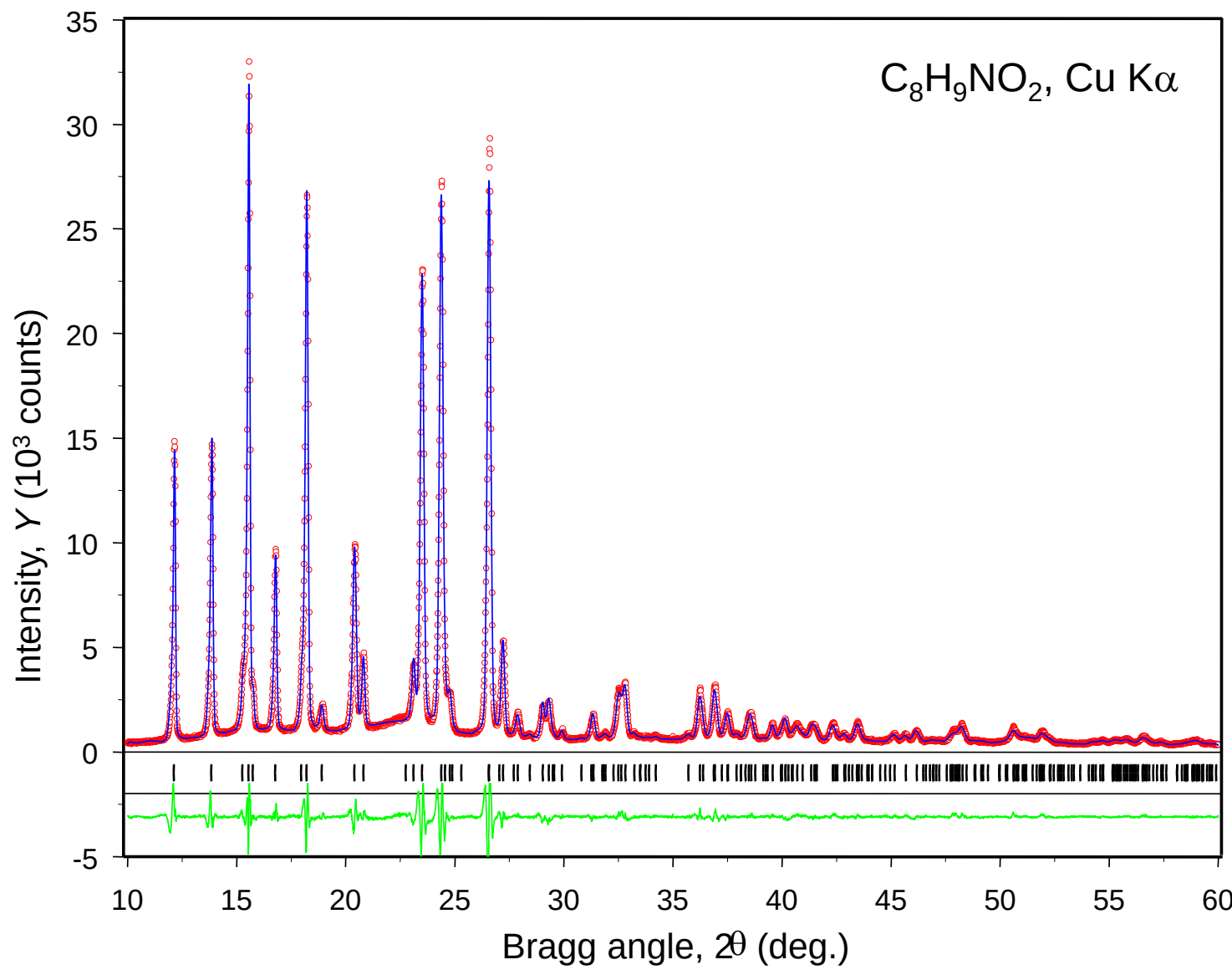
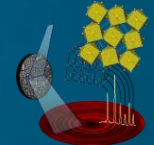


Figure 25.8. The results of the Rietveld refinement of the acetaminophen structure using GSAS, showing the observed (*red circles*) and calculated (*blue solid line*) diffraction patterns. The *vertical bars* indicate the positions of the $K\alpha_1$ components of the calculated Bragg peaks. The line at the *bottom* shows the difference between the observed and calculated profiles.

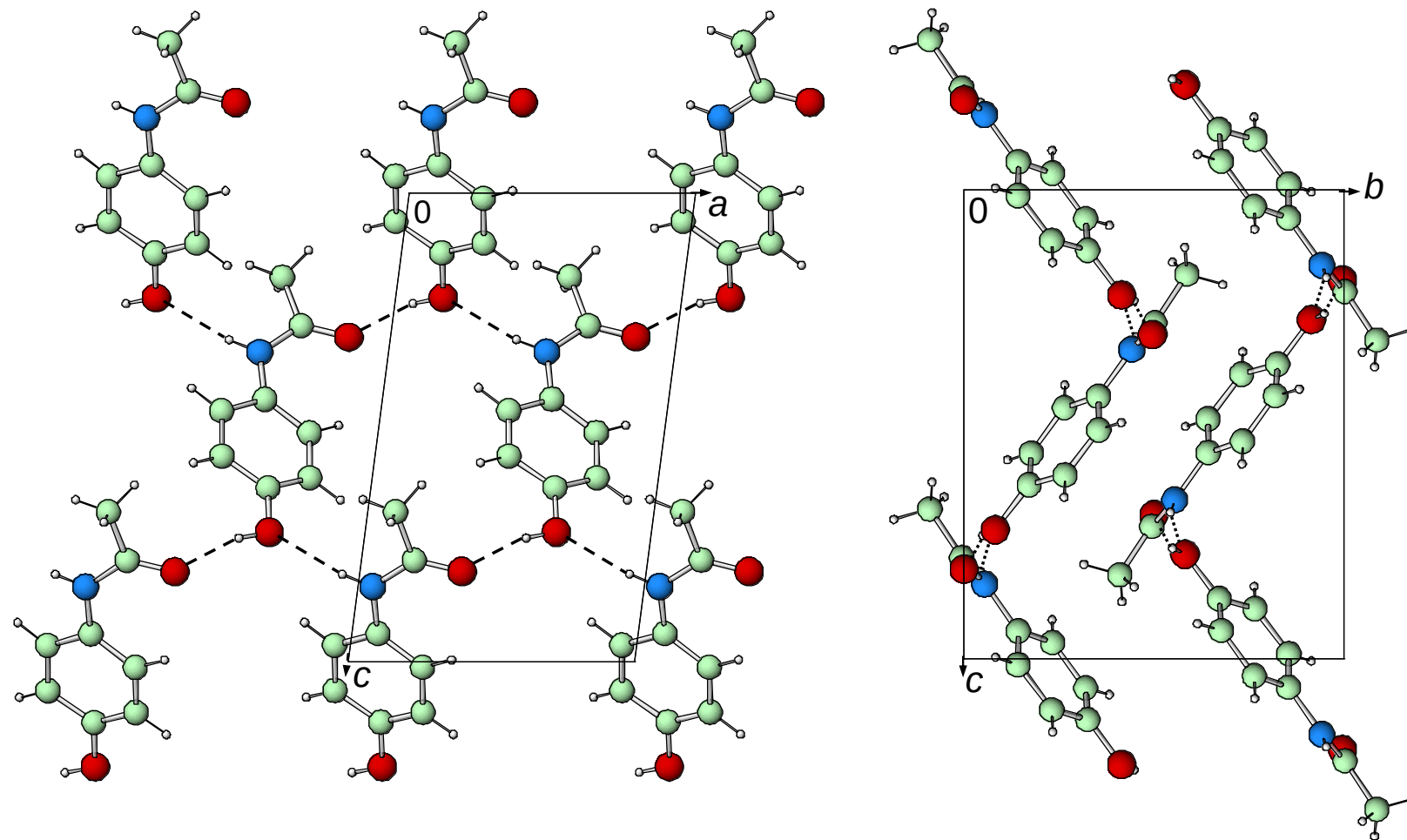
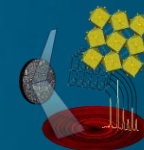


Figure 25.9. The layer of H-bonded acetaminophen molecules (*left*) and the packing of zigzag layers (*right*). Oxygen atoms are *red*, nitrogen *blue*, and carbon *green*. Hydrogen atoms are depicted as *small white circles* and hydrogen bonds as *dotted lines*.

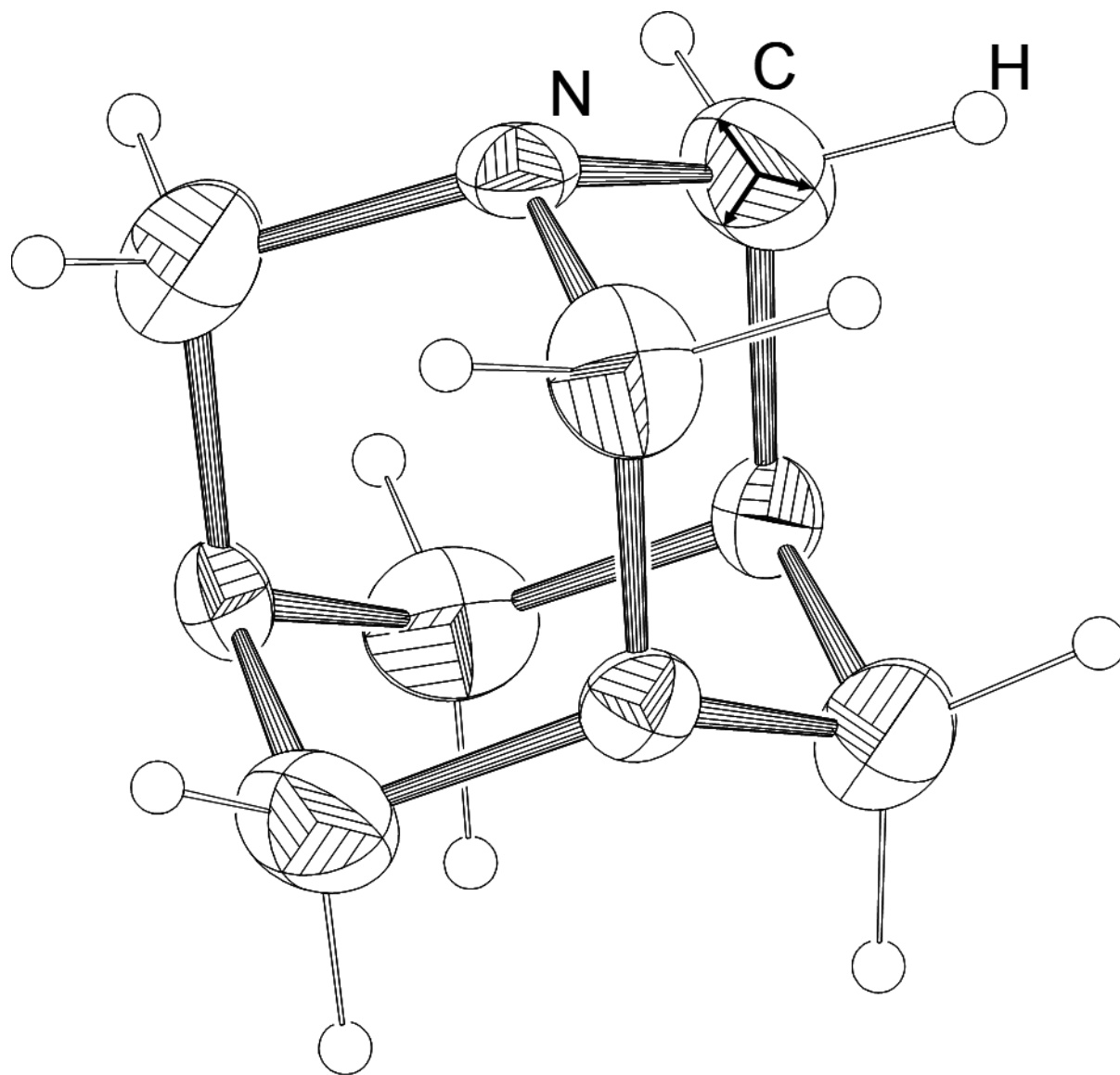
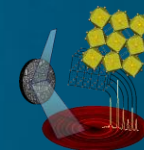


Figure 25.10. The molecule of hexamethylenetetramine, shown using displacement ellipsoids of carbon and nitrogen atoms.