and 18-electron complexes, respectively. Crystal formation refinement. refinements, based on F2 with applied extinction correction. For all compounds studied that was ligands that clue to the different size of the ligand ring the energy interaction with the A. radiation up to 0.2 eÅ−3 and 0.3 eÅ−3 directed between the vertices of the octahedron.

New X-ray diffraction data for adenine complexes (C8H6N4O2) have been collected at high resolution (sinθ/λ < 1.34Å−1) and reduced temperature (123K). The structure has been refined by least squares using Stewart’s rigid pseudotetramer model. All nuclear positional and anisotropic m.s. displacement parameters were assigned fixed values from a previous neutron diffraction study at 123K (1). Thus the least squares refinement involved only the scale factor, an isotropic extinction parameter, three X radial parameters (for C, N and O), and 356 pseudotetramer electron population parameters. The refinement, which was based on F2 and included all 10,083 reflections, gave R(F2) = 0.046 and Rw(F2) = 0.077 with goodness-of-fit = 1.64.

The total electronic charge density in the crystal p(r), has been mapped for pseudotetramers at rest. Also the Laplacian of the charge density Vp(r) has been analysed at the (3, -1) bond critical points (2). At the bond critical points, p(r) is consistently greater in the adenine base than in the ribose sugar. Thus C4-C5 and C5-C6 in adenine ring system have p(r) = 2.05(7), 2.02(7)eÅ−3, whereas C1’-C2’ and C2’-C3’ in the ribose ring have p(r) = 1.78(6), 1.67(5)eÅ−3. Also, the Hessian matrix at the bond critical points indicates considerable double bond character for C4-C5 and C5-C6 (ie 0.43, 0.43) whereas this is lacking for C1’-C2’ and C2’-C3’ (ε = 0.09, 0.12). The Laplacian at all H-bond critical points is positive, indicating a lack of covalent bonding. There is a week H bond, C2-H2...O2.

Work supported by a grant GM-39513 from NIH.