X-ray studies of such a series of adenine derivatives are thus appropriate for deducing structure-activity relationships of cytokinins. The structures of derivatives, n=0, 2 and 3 were solved by MULTAN 84. The most interesting feature is an alternation of the values of interplanar angle between purine and phenyl ring system. Those angles in active derivatives (n=even) are fairly close to 30° as observed in other active cytokinins, whereas about 30° in weakly active derivatives (n=odd) are closely related to cytokinin activity and can be correlated with the crystal structure. The conformations of the ring systems and the spatial orientation of the -CH=CH₂ substituent on nitrogen will be compared with those found in a series of related agonist and antagonist molecules. Possible implications for biological activity will be considered.