The structures of 1,4-benzodiazepines were determined by the X-ray method. In all three cases the structures are molecular ones. The structure (I) is built up of molecular dimers by two intramolecular H-bonds. The molecule consists of nearly flat fragments with "bath" conformation. The 16-membered heterocycle contains a C₃₆-axis and is stabilized by two intramolecular H-bonds. The molecule consists of nearly flat fragments with "bath" conformation.