

However, as illustrated in Figure 0637, two adjacent equatorial groups can experience an additional gauche interaction between them (case i), two axial groups on the same face of a molecule can experience additional steric hindrance called a 1,3-diaxial interaction (case ii), two electronegative atom groups can experience 1,3-diaxial repulsion plus an additional charge/charge repulsion (case iii), and in case iv, the two axial groups have 1,3-diaxial repulsion plus a charge/charge repulsion, but this is counteracted by an intramolecular hydrogen bond that can help stabilize the diaxial conformation (because they can reach each other when they are both axial and on the same side, but not when they are equatorial). In all of these cases, additional experimental information would be required to estimate the energy difference between the two chair conformations.

Figure 0637

Some disubstituted cyclohexanes where A-Values alone cannot be used reliably.

