out-of-plane bending coordinate

in molecular geometry

Given by

\[ \Delta \theta_{i-jkl} = \frac{\Delta z_j}{r_{eij}} \sin \Phi_{kil} \]

where the numbering of the atoms is given in the diagram. \( \Phi_{kil} \) denotes the angle between the bonds \( ik \) and \( il \), \( \Delta z_j \) the perpendicular distance of the atom \( j \) from the instantaneous plane \( ikl \) and \( r_{eij} \) the equilibrium length of the bond \( ij \).

Source:
PAC, 1978, 50, 1707 (Definition and symbolism of molecular force constants) on page 1710