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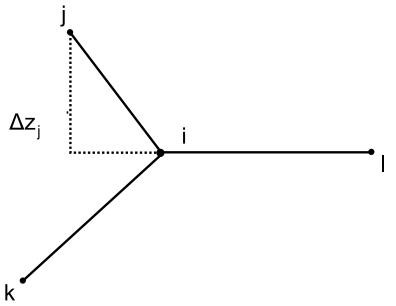
out-of-plane bending coordinate

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. Φ_{kil} denotes



the angle between the bonds *ik* and *il*, Δz_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

