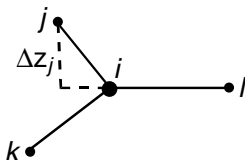


### out-of-plane bending coordinate (in molecular geometry)

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  $ij$ .

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