

general force field (gff)

A force field expressed in terms of $3N - 6$ basis coordinates:

$$V = \frac{1}{2} \sum f_{ij} \text{ (or } F_{ij}) S_i S_j$$

where f_{ij} (or F_{ij}) are force constants and the basis coordinates S (or sometimes s) may be internal symmetry coordinates, local symmetry coordinates or any others suitable to the problem, but the number of the coordinates has to be reduced to $3N - 6$ ($3N - 5$ for linear molecules), N being the number of atoms in the molecule.

1978, 50, 1709