

## general force field

**Acronym:** gff

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

$$V = \frac{1}{2} \sum f_{ij} S_i S_j$$

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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.

**Source:**

PAC, 1978, 50, 1707 (*Definition and symbolism of molecular force constants*) on page 1709