

## Cut-Off

- **KA** (Keep All). All elements in matrices for algebraic forms are taken into consideration.
- **LG**. The *lag* assumes values between 1 and L. The idea of a *lag* is taken from autocorrelation descriptors, only that here the meaning is quite different. This cutoff is applied to the elements in the matrices for the algebraic forms, namely NS, SS and MP. In this software, a range of k values will be used instead of only one value of k, *e.g.*, k= 2-5, k=2;4;7-9.
  - **LG[p]** (lag p). In this *lag* the maximum value L can be  $n - 1$ , where n is the number of atoms. When this lag is applied, the matrix elements are different from zero for relations of atoms that have at less an atom-pair with *topological distance*, *p*, equal to a specified *k* value.
  - **LG[l]** (lag l). In this *lag* the maximum value L will be less than the maximum Euclidean distance between two atoms. When this lag is applied, the matrix elements are different from zero for relations of atoms that have at less an atom-pair with *geometrical Euclidean distance*, *l*, less or equal to a specified *k* value.