Cut-Off

- **KA** (Keep All). All elements in matrices for algebraic forms are taken into consideration.
- **SRW** (Self-Returning Walk). Here only diagonal elements of algebraic forms matrices are taken into account.
- **NSWR** (Non Self-Returning Walk). Here only off-diagonal elements of algebraic forms matrices are taken into account.
- **LG[p]** (lag p). The *lag* assumes values between 1 and L, where the maximum value L can be n - 1. However, in several applications, L is a small number (L < 8). The idea of a *lag* is taken from autocorrelation descriptors,(Broto and Devillers 1990) 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, DS and MP. If lag k is used, the matrix elements are different from zero for pairs of atoms that have a *topological distance, d,* equal to a specified *k* value. That is to say, the number of vertex pairs at distance equal to *d.* However, 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.