APPENDIX K: WHEN TO DROP NONOBSERVABLE TERMS (NOT)

In the expression of the density matrix we are interested in those POs which represent observable magnetization components: M_x and M_y for the nucleus (or nuclei) which are observed (see Appendix J). We have to carry all the nonobservable terms through the calculations as long as there is a possibility for them to generate observable terms (following a pulse or an evolution).

It is useful to be aware when it is safe to drop the nonobservable terms, or just include them in the nondescript designation NOT.

Rule #1. In the final expression $D(n)$ of the density matrix we have to write down explicitly the observable terms only for the specific nucleus which is observed. This includes the POs which show x or y for the observed nucleus and 1 for all others.

Rule #2. A decoupled evolution does not generate observable POs out of NOT or the reverse: it merely replaces x by y or y by $-x$. So, if the last event of the sequence (the detection) is a decoupled evolution, we can do the selection earlier, when writing $D(n-1)$.

Rule #3. A coupled evolution can interchange x and y but also 1 and z. Although, we can do some term dropping before the last evolution, even if coupled. In writing $D(n-1)$ we will retain only the POs which contain x or y for the nucleus to be observed and z or 1 for the other nuclei. Everything else is a NOT.

For instance, if we observe nucleus A (in an AMX system), the following terms must be kept:

$$[x11],\ [x1z],\ [xz1],\ [xzz],\ [y11],\ [y1z],\ [yz1],\ [yzz].$$

Note. If a pulse still follows, it is recommended to use utmost care in dropping terms. An experienced student will find for example that if the observable is A and the last pulse is on X, terms like [1x], [1z], [zx], (no x or y in position A) can be labeled as NOT before the pulse since an X pulse will never render them observable.