APPENDIX C: ANGULAR MOMENTUM AND ROTATION OPERATORS

System (spin): A(1/2)

$$I_x = \frac{1}{2}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \quad ; \quad I_y = \frac{1}{2}\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \tag{C1}$$

$$I_z = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad ; \quad I_x + iI_y = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \tag{C2}$$

$$R_{\alpha x} = \begin{bmatrix} \cos\frac{\alpha}{2} & i\sin\frac{\alpha}{2} \\ i\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{bmatrix} \; ; \; R_{\alpha y} = \begin{bmatrix} \cos\frac{\alpha}{2} & \sin\frac{\alpha}{2} \\ -\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{bmatrix} \tag{C3}$$

$$R_{90x} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix} \quad ; \quad R_{90y} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \tag{C4}$$

$$R_{180x} = \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix} \quad ; \quad R_{180y} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \tag{C5}$$

System (spin): A(1)

$$I_x = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad ; \quad I_y = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix} \tag{C6}$$

$$I_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix} \; ; \; I_x + iI_y = \sqrt{2}\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \tag{C7}$$

$$R_{\alpha x} = \frac{1}{2}\begin{bmatrix} \cos\alpha + 1 & i\sqrt{2}\sin\alpha & \cos\alpha - 1 \\ i\sqrt{2}\sin\alpha & 2\cos\alpha & i\sqrt{2}\sin\alpha \\ \cos\alpha - 1 & i\sqrt{2}\sin\alpha & \cos\alpha + 1 \end{bmatrix} \tag{C8}$$

$$R_{\alpha y} = \frac{1}{2}\begin{bmatrix} 1+\cos\alpha & \sqrt{2}\sin\alpha & 1-\cos\alpha \\ -\sqrt{2}\sin\alpha & 2\cos\alpha & \sqrt{2}\sin\alpha \\ 1-\cos\alpha & -\sqrt{2}\sin\alpha & 1+\cos\alpha \end{bmatrix} \qquad \text{(C9)}$$

$$R_{90x} = \frac{1}{2}\begin{bmatrix} 1 & i\sqrt{2} & -1 \\ i\sqrt{2} & 0 & i\sqrt{2} \\ -1 & i\sqrt{2} & 1 \end{bmatrix} \; ; \; R_{90y} = \frac{1}{2}\begin{bmatrix} 1 & \sqrt{2} & 1 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{bmatrix} \text{(C10)}$$

$$R_{180x} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix} \quad ; \quad R_{180y} = \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \qquad \text{(C11)}$$

System (spin): A(1/2) X(1/2)

$$I_{xA} = \frac{1}{2}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \quad ; \quad I_{yA} = \frac{1}{2}\begin{bmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{bmatrix} \quad \text{(C12)}$$

$$I_{zA} = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} ; (I_x + iI_y)_A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{(C13)}$$

$$I_{xX} = \frac{1}{2}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} ; \qquad I_{yX} = \frac{1}{2}\begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{bmatrix} \text{(C14)}$$

$$I_{zX} = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}; (I_x + i\, I_y)_X = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \text{(C15)}$$

$$R_{90xA} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & i & 0 & 0 \\ i & 1 & 0 & 0 \\ 0 & 0 & 1 & i \\ 0 & 0 & i & 1 \end{bmatrix}; \quad R_{90yA} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 \end{bmatrix} \quad \text{(C16)}$$

$$R_{180xA} = \begin{bmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \end{bmatrix}; \quad R_{180yA} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{bmatrix} \quad \text{(C17)}$$

$$R_{90xX} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & i & 0 \\ 0 & 1 & 0 & i \\ i & 0 & 1 & 0 \\ 0 & i & 0 & 1 \end{bmatrix}; \quad R_{90yX} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix} \quad \text{(C18)}$$

$$R_{180xX} = \begin{bmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{bmatrix}; \quad R_{180yX} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} \quad \text{(C19)}$$

Examples of *selective* rotation operators, affecting only one of the two possible transitions of nucleus X: 2-4 or 1-3.

$$R_{90x(24)} = \frac{1}{\sqrt{2}}\begin{bmatrix} \sqrt{2} & 0 & 0 & 0 \\ 0 & 1 & 0 & i \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & i & 0 & 1 \end{bmatrix}; R_{90y(24)} = \frac{1}{\sqrt{2}}\begin{bmatrix} \sqrt{2} & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & -1 & 0 & 1 \end{bmatrix}$$

(C20)

$$R_{180x(24)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 1 & 0 \\ 0 & i & 0 & 0 \end{bmatrix} \; ; \; R_{180y(24)} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix} \quad \text{(C21)}$$

$$R_{90x(13)} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & i & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ i & 0 & 1 & 0 \\ 0 & 0 & 0 & \sqrt{2} \end{bmatrix} ; R_{90y(13)} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & \sqrt{2} \end{bmatrix}$$

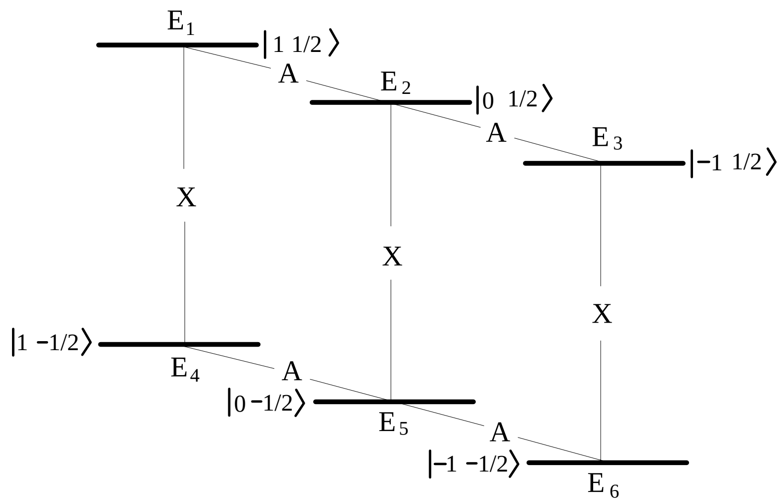
(C22)

$$R_{180x(13)} = \begin{bmatrix} 0 & 0 & i & 0 \\ 0 & 1 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \; ; \; R_{180y(13)} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad \text{(C23)}$$

Selective rotation operators for the nucleus A (transition 1-2 or 3-4) can be written in a similar manner.

System (spin): A(1) X(1/2)

The energy states are labeled according to the figure below.



$$I_{xA} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{bmatrix} \qquad \text{(C24)}$$

$$I_{xX} = \frac{1}{2} \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix} \qquad \text{(C25)}$$

I_y can be written in the same way, taking (C6) and (C1) as starting points.

Examples of rotation operators for the AX(1, 1/2) system:

$$R_{90yA} = \frac{1}{2}\begin{bmatrix} 1 & 0 & \sqrt{2} & 0 & 1 & 0 \\ 0 & 1 & 0 & \sqrt{2} & 0 & 1 \\ -\sqrt{2} & 0 & 1 & 0 & \sqrt{2} & 0 \\ 0 & -\sqrt{2} & 0 & 1 & 0 & \sqrt{2} \\ 1 & 0 & -\sqrt{2} & 0 & 1 & 0 \\ 0 & 1 & 0 & -\sqrt{2} & 0 & 1 \end{bmatrix} \qquad \text{(C26)}$$

$$R_{180xX} = \begin{bmatrix} 0 & i & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i & 0 & 0 \\ 0 & 0 & i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 & i & 0 \end{bmatrix} \qquad \text{(C27)}$$

Reciprocals R^{-1} of all rotation operators can be found through transposition and complex conjugation (see Appendix A).

Rotations about the z-axis

These rotation operators are needed in the following section (Phase Cycling). They can be derived in the same way as the *x* and *y* rotation operators [see (B45) to (B54)], after observing that

$$I_z^n = \left(\frac{1}{2^n}\right)\cdot[1] \qquad \text{for n=even}$$

$$I_z^n = \left(\frac{1}{2^n}\right)\cdot(2I_z) \qquad \text{for n=odd} \qquad \text{(C28)}$$

For the one spin system A(1/2) we have

$$R_{\alpha z} = \begin{bmatrix} b & 0 \\ 0 & b^* \end{bmatrix} \qquad \text{(C29)}$$

with $$b = \cos(\alpha/2) + i\sin(\alpha/2) = \exp(i\alpha/2) \quad \text{(C30)}$$

For the two spin system A(1/2)X(1/2) we have

$$R_{\alpha zA} = \begin{bmatrix} b & 0 & 0 & 0 \\ 0 & b^* & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & b^* \end{bmatrix} ; \; R_{\alpha zX} = \begin{bmatrix} b & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & b^* & 0 \\ 0 & 0 & 0 & b^* \end{bmatrix} \quad \text{(C31)}$$

$$R_{\alpha zAX} = R_{\alpha zA} R_{\alpha zX} = \begin{bmatrix} b^2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & b^{*2} \end{bmatrix} \quad \text{(C32)}$$

Phase cycling

This section contains rotation operators for phase cycled pulses. The rotation axis for such pulses is situated in the *xy* plane and makes an angle Φ with the *x*-axis. In succesive runs, the angle Φ assumes different values. When Φ is equal to 0°, 90°, 180°, or 270°, the rotation axis is *x*, *y*, $-x$, or $-y$, respectively. The expressions given in this section are valid for any value of Φ, even if it is not a multiple of 90°. Such values are seldom used in pulse sequences but they may be used to assess the effect of imperfect phases.

The rotation operator R_{90} represents a 90° rotation about an axis making the angle Φ with the *x*-axis. In order to find the expression of R_{90}, we observe that this rotation is equivalent with the following succession of rotations:

a. A rotation by $-\Phi$ (clockwise) about *Oz*, bringing the rotation axis in line with *Ox*.
b. A 90° rotation about *Ox*.
c. A rotation by Φ (counterclockwise) about *Oz*.

For the one-spin system A(1/2), using (C29), this leads to

$$R_{90\Phi} = R_{(-\Phi)z} R_{90x} R_{\Phi z}$$

$$= \begin{bmatrix} b^* & 0 \\ 0 & b \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix} \begin{bmatrix} b & 0 \\ 0 & b^* \end{bmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{bmatrix} b^* & 0 \\ 0 & b \end{bmatrix} \begin{bmatrix} b & ib^* \\ ib & b^* \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & ib^{*2} \\ ib^2 & 1 \end{bmatrix} \tag{C33}$$

where $b = \exp(i\Phi/2)$ from (C30). With the new notation

$$a = ib^{*2} = i\exp(-i\Phi) \tag{C34}$$

the relation (C33) becomes

$$R_{90\Phi} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & a \\ -a^* & 1 \end{bmatrix} \tag{C35}$$

In a similar way one can demonstrate that

$$R_{180\Phi} = \begin{bmatrix} 0 & a \\ -a^* & 0 \end{bmatrix} \tag{C36}$$

For the two-spin system A(1/2)X(1/2)

$$R_{90\Phi A} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & a & 0 & 0 \\ -a^* & 1 & 0 & 0 \\ 0 & 0 & 1 & a \\ 0 & 0 & -a^* & 1 \end{bmatrix} \tag{C37}$$

$$R_{90\Phi X} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & a & 0 \\ 0 & 1 & 0 & a \\ -a^* & 0 & 1 & 0 \\ 0 & -a^* & 0 & 1 \end{bmatrix} \tag{C38}$$

$$R_{90\Phi AX} = R_{90\Phi A} R_{90\Phi X} = \frac{1}{2} \begin{bmatrix} 1 & a & a & a^2 \\ -a^* & 1 & -1 & a \\ -a^* & -1 & 1 & a \\ a^{*2} & -a^* & -a^* & 1 \end{bmatrix} \tag{C39}$$

This operator has been used in the DM treatment of INADEQUATE [see (I.83)].

One can verify that for $\Phi = 0$ we have $a = i$ and

$$R_{90\Phi AX} = R_{90xAX} \qquad \text{[cf.(I.34)]}$$

When $\Phi = 90^o$ we have $a = 1$ and

$$R_{90\Phi AX} = R_{90yAX} \qquad \text{[cf.(I.101)]}$$

For the 180^o pulse, similar calculations lead to

$$R_{180\Phi A} = \begin{bmatrix} 0 & a & 0 & 0 \\ -a* & 0 & 0 & 0 \\ 0 & 0 & 0 & a \\ 0 & 0 & -a* & 0 \end{bmatrix} \qquad (C40)$$

$$R_{180\Phi X} = \begin{bmatrix} 0 & 0 & a & 0 \\ 0 & 0 & 0 & a \\ -a* & 0 & 0 & 0 \\ 0 & -a* & 0 & 0 \end{bmatrix} \qquad (C41)$$

$$R_{180\Phi AX} = \begin{bmatrix} 0 & 0 & 0 & a^2 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ a*^2 & 0 & 0 & 0 \end{bmatrix} \qquad (C42)$$

The 180^o operators can be calculated by multiplying the respective 90^o operator with itself (two successive 90^o rotations).

Cyclops

Even in the simplest one-dimensional sequences, involving one single pulse (the "observe" pulse), a form of phase cycling is used in order to eliminate the radiofrequency interferences. The observe pulse is cycled through all four phases, e.g. clockwise: +x, − y, − x, +y. The f.i.d. phase follows the same pattern. There will be no accumulation unless the reciever phase is also cycled clockwise. An extraneous signal is not phase cycled and it will be averaged out because of the receiver cycling, provided the number of transients is a multiple of four. The procedure is known as "cyclops".