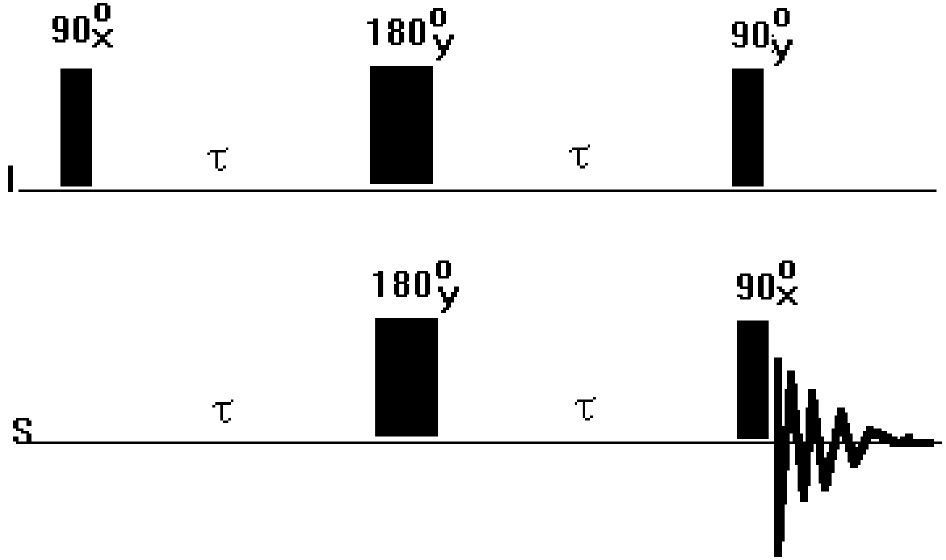
INEPT = Insensitive Nuclei Enhanced by Polarization Transfer

Heteronuclear I, S
Consider: Ω_I, Ω_S and J_{IS}
(I and S are heteronuclear)



The pulse sequence:

(e.g.^{1}H)	I:	$90°_x$ -----τ----- $180°_y$ ------τ-----$90°_y$
(e.g.^{13}C)	S:	-----τ----- $180°_y$ ------τ-----$90°_x$ACQ
		-----------e c h o ------------

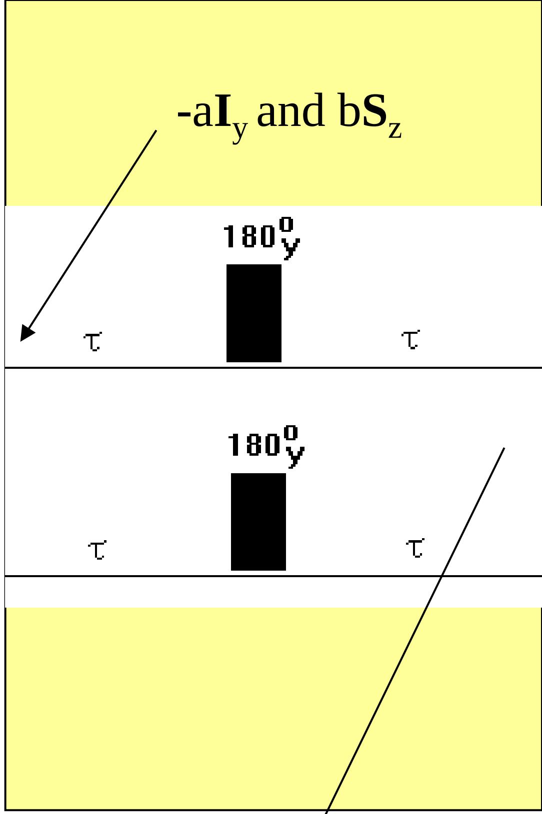
$\tau = 1/(4J_{IS})$ e.g. J_{CH}= 150 Hz -> τ = 1.67 ms

a≅4b (the intensity (γ) difference between spin I and S)

σ[eq.]	a$\mathbf{I}_z$ and b$\mathbf{S}_z$
$\hat{H} = \pi/2\ (\hat{I}_x)$	↓$90°_x$
σ[0]	-a$\mathbf{I}_y$ and b$\mathbf{S}_z$

memo : this is a spin-echo ***(180º on I and S „homo”-like situation)***

coupling evolves but chemical shift doesn't evolve



$\hat{H} = 2\hat{I}_z\check{S}_z(J_{IS}\pi\tau)$ $\downarrow$

$-a\mathbf{I}_y \cos(\pi J_{IS}\tau)$

$+a2\mathbf{I}_x\mathbf{S}_z \sin(\pi J_{IS}\tau)$

$b\mathbf{S}_z$

$\hat{H} = \pi\hat{I}_y$ $\downarrow$

$-a\mathbf{I}_y \cos(\pi J_{IS}\tau)$

$-a2\mathbf{I}_x\mathbf{S}_z \sin(\pi J_{IS}\tau)$

$b\mathbf{S}_z$

$\hat{H} = \pi S_y$ $\downarrow$

$-a\mathbf{I}_y \cos(\pi J_{IS}\tau)$

$+a2\mathbf{I}_x\mathbf{S}_z \sin(\pi J_{IS}\tau)$

$-b\mathbf{S}_z$

$\hat{H} = 2\hat{I}_z\check{S}_z(J_{IS}\pi\tau)$ $\downarrow$

$-a\mathbf{I}_y \cos(\pi J_{IS}\tau)\cos(\pi J_{IS}\tau)$

$+a2\mathbf{I}_x\mathbf{S}_z \cos(\pi J_{IS}\tau)\sin(\pi J_{IS}\tau)$

$+a2\mathbf{I}_x\mathbf{S}_z \sin(\pi J_{IS}\tau)\cos(\pi J_{IS}\tau)$

$+a\mathbf{I}_y \sin(\pi J_{IS}\tau)\sin(\pi J_{IS}\tau)$

$-b\mathbf{S}_z$

memo 1: /$\cos^2 A - \sin^2 A = \cos 2A$*/*

$-a\mathbf{I}_y \{\cos(\pi J_{IS}\tau)\cos(\pi J_{IS}\tau) - \sin(\pi J_{IS}\tau)\sin(\pi J_{IS}\tau)\} = -a\mathbf{I}_y \cos(2\pi J_{IS}\tau)$

memo 2: /$2\cos A \sin A = \sin 2A$*/*

$2\{+a2\mathbf{I}_x\mathbf{S}_z \sin(\pi J_{IS}\tau)\cos(\pi J_{IS}\tau)\} = +a2\mathbf{I}_x\mathbf{S}_z \sin(2\pi J_{IS}\tau)$

Therefore the $-a\mathbf{I}_y \cos(2\pi J_{IS}\tau)$ $+a2\mathbf{I}_x\mathbf{S}_z \sin(2\pi J_{IS}\tau)$ $-b\mathbf{S}_z$ terms remain.

since $\tau = 1/(4J_{IS})$ ----> $\cos(2\pi J_{IS}\tau)=0$ and $\sin(2\pi J_{IS}\tau)=1$

Phase cycling starts here

	$+a2\mathbf{I}_x\mathbf{S}_z$ $-b\mathbf{S}_z$	
$\hat{H} = \pi/2 \ (\hat{I}_{\pm y})$	$\downarrow 90°_{+y}$	$\downarrow 90°_{-y}$
	$-a2\mathbf{I}_z\mathbf{S}_z$ $-b\mathbf{S}_z$	$+a2\mathbf{I}_z\mathbf{S}_z$ $-b\mathbf{S}_z$
$\hat{H} = \pi/2 \ (S_x)$	$\downarrow 90°_x$	$\downarrow 90°_x$
	$+a2\mathbf{I}_z\mathbf{S}_y$ $+b\mathbf{S}_y$	$-a2\mathbf{I}_z\mathbf{S}_y$ $+b\mathbf{S}_y$

Both terms are magnetization on spin S

1) $+a2\mathbf{I}_z\mathbf{S}_y$: anti-phased magnetization on spin S with intensity factor of spin I.

2) $+b\mathbf{S}_y$: in phased magnetization on spin S.

The first term during ACQ : $+a2\mathbf{I}_z\mathbf{S}_y$

$\hat{H} = S_z(\Omega_S[t_2])$
$\hat{H} = 2\hat{I}_z\check{S}_z(J_{IS}\pi[t_2])$

$\downarrow$

$$+a2\mathbf{I}_z\mathbf{S}_y \cos(\Omega_S t_2)\cos(\pi J_{IS} t_2)$$
$$-a\mathbf{S}_x \cos(\Omega_S t_2)\sin(\pi J_{IS} t_2)$$
$$-a2\mathbf{I}_z\mathbf{S}_x \sin(\Omega_S t_2)\cos(\pi J_{IS} t_2)$$
$$-a\mathbf{S}_y \sin(\Omega_S t_2)\sin(\pi J_{IS} t_2)$$

memo 1: put the receiver on x
therefore only the single x term remain : $-a\mathbf{S}_x\cos(\Omega_S t_2)\sin(\pi J_{IS} t_2)$

memo 2: cos(A)sin(B) = 1/2[sin(A+B)-sin(A-B)]
therefore $-a\mathbf{S}_x 1/2[+\sin\{(\Omega_S+\pi J_{IS})t_2\}- \sin\{(\Omega_S-\pi J_{IS})t_2\}]$

the following terms can be found: $-\ a\mathbf{S}_x$ 1/2[+ .... - ....] at Ω_S

setting the phase that *sin* is absorptive : $-a\mathbf{S}_x$ 1/2[+a .. -a ..] at Ω_S

remark: an antiphase doublet ($^{1,1}J$[H,N] ≅90 Hz, $^{1,1}J$[H,C] ≅150 Hz) is observed.
conclusion: The spectrum is an antiphase doublet at Ω_S of an **enhanced intensity**.

The second term during ACQ : $+b\mathbf{S}_y$

$\hat{H} = S_z(\Omega_S[t_2])$

$\hat{H} = 2\hat{I}_z\check{S}_z(J_{IS}\pi[t_2])$

$\downarrow$

$+b\mathbf{S}_y \cos(\Omega_S t_2)\cos(\pi J_{IS} t_2)$

$-b2\mathbf{I}_z\mathbf{S}_x \cos(\Omega_S t_2)\sin(\pi J_{IS} t_2)$

$-b\mathbf{S}_x \sin(\Omega_S t_2)\cos(\pi J_{IS} t_2)$

$-b2\mathbf{I}_z\mathbf{S}_y \sin(\Omega_S t_2)\sin(\pi J_{IS} t_2)$

memo 1: we placed the receiver on x

therefore only the single x term remains: $-b\mathbf{S}_x \sin(\Omega_S t_2)\cos(\pi J_{IS} t_2)$

memo 2: sin(A)cos(B) = 1/2[sin(A+B) + sin(A-B)]

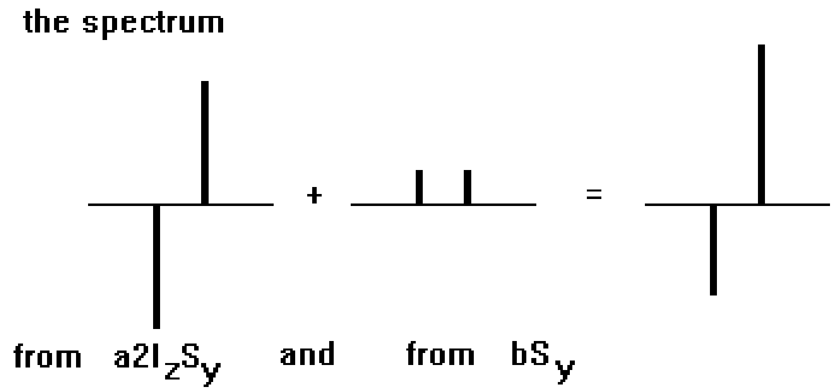
therefore $-b\mathbf{S}_x 1/2[+\sin\{(\Omega_S+\pi J_{IS})t_2\} + \sin\{(\Omega_S-\pi J_{IS})t_2\}]$

the following terms can be found: $-\ b\mathbf{S}_x$ 1/2[+ .... + ...] at Ω_S

we have set the phase that *sin* is absorptive : $-b\mathbf{S}_x$ 1/2[+a .. +a ..] at Ω_S

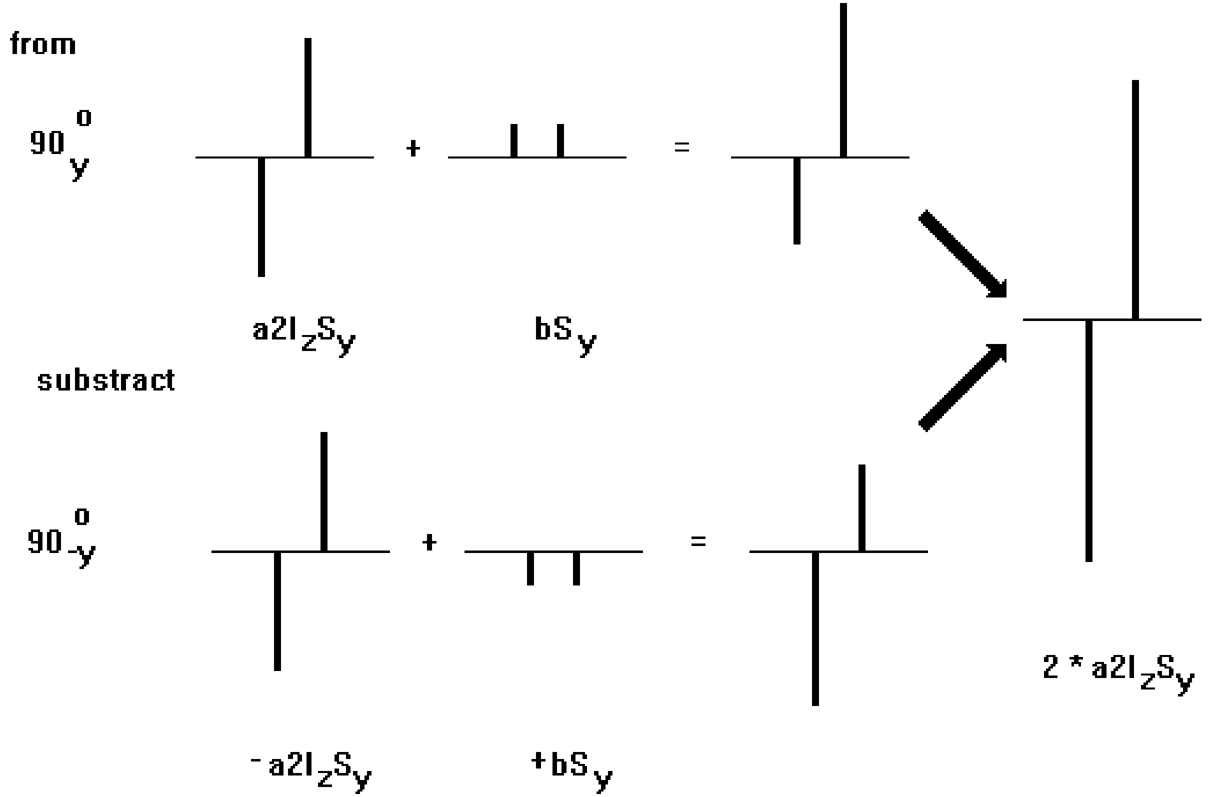
the two terms are the following:

$-a\mathbf{S}_x 1/2[+\sin\{(\Omega_S+\pi J_{IS})t_2\} - \sin\{(\Omega_S-\pi J_{IS})t_2\}]$
$-b\mathbf{S}_x 1/2[+\sin\{(\Omega_S+\pi J_{IS})t_2\} + \sin\{(\Omega_S-\pi J_{IS})t_2\}]$



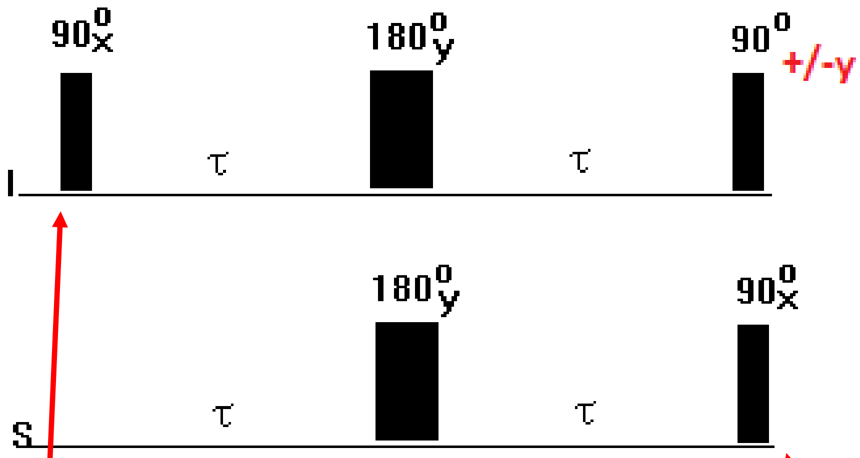
The second term
can be phase-cycled out
(2 step phase cycle).

Therefore, the two
$+a2\mathbf{I}_z\mathbf{S}_y$ remain.



What does the INEPT module?

Heteronuclear I, S,
with Ω_I, Ω_S and J_{IS}



after phase cycling

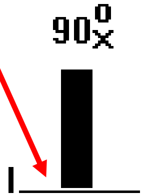
$a\mathbf{I}_z$

$\pm a2\mathbf{I}_z\mathbf{S}_y$

anti-phase S

An INEPT module makes from in-phased I an anti-phased S coherence. But with the coherence transfer „the sensitivity (a)"of spin I is also transferred!!!

Compare to a simple 90_x°:



$-a\mathbf{I}_y$ **in-phase I**