



J | A | C | S
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

J. Am. Chem. Soc., 1998, 120(41), 10778-10779, DOI: [10.1021/ja982649y](https://doi.org/10.1021/ja982649y)

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at <http://pubs.acs.org/page/copyright/permissions.html>



ACS Publications

MOST TRUSTED. MOST CITED. MOST READ.

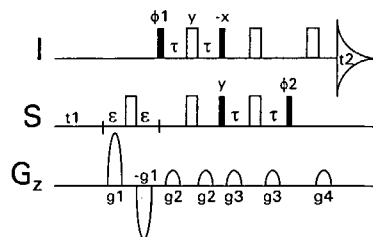
Copyright © 1998 American Chemical Society

Supporting Information to:**“Single Scan, Sensitivity- and Gradient-Enhanced TROSY for Multidimensional NMR Experiments”**

Johan Weigelt

Cartesian product operator¹ analysis of the following pulse sequence element to select different subspectra

Pulse sequence:



gradients labeled g1 and g4 of equal length

$$\tau = 1/4J_{IS}$$

$$J_{IS} < 0$$

Terms present by the end of t_1 : ²		$\cos(\omega_S t_1) \cos(\pi J_{IS} t_1) 2S_x I_z + \sin(\omega_S t_1) \cos(\pi J_{IS} t_1) 2S_y I_z + \cos(\omega_S t_1) \sin(\pi J_{IS} t_1) S_y - \sin(\omega_S t_1) \sin(\pi J_{IS} t_1) S_x$				
Experiment ³	g1	ϕ_1	ϕ_2	Terms present at the start of t_2	Add = A + B Subtract = A - B ^{4, 5}	Subspectrum
1A	$ \gamma_I/2\gamma_S g_4$	y	x	$-0.5\sin((\omega_S - \pi J_{IS})t_1)(I_x + 2I_x S_z) - 0.5\cos((\omega_S - \pi J_{IS})t_1)(I_y + 2I_y S_z)$	$-\sin((\omega_S - \pi J_{IS})t_1)(I_x + 2I_x S_z)$	o o
1B	$- \gamma_I/2\gamma_S g_4$	-y	-x	$-0.5\sin((\omega_S - \pi J_{IS})t_1)(I_x + 2I_x S_z) + 0.5\cos((\omega_S - \pi J_{IS})t_1)(I_y + 2I_y S_z)$	$-\cos((\omega_S - \pi J_{IS})t_1)(I_y + 2I_y S_z)$	o x
2A	$ \gamma_I/2\gamma_S g_4$	-y	-x	$0.5\sin((\omega_S + \pi J_{IS})t_1)(I_x - 2I_x S_z) + 0.5\cos((\omega_S + \pi J_{IS})t_1)(I_y - 2I_y S_z)$	$\sin((\omega_S + \pi J_{IS})t_1)(I_x - 2I_x S_z)$	x o
2B	$- \gamma_I/2\gamma_S g_4$	y	x	$0.5\sin((\omega_S + \pi J_{IS})t_1)(I_x - 2I_x S_z) - 0.5\cos((\omega_S + \pi J_{IS})t_1)(I_y - 2I_y S_z)$	$\cos((\omega_S + \pi J_{IS})t_1)(I_y - 2I_y S_z)$	o o
3A	$ \gamma_I/2\gamma_S g_4$	y	-x	$-0.5\sin((\omega_S - \pi J_{IS})t_1)(I_x - 2I_x S_z) - 0.5\cos((\omega_S - \pi J_{IS})t_1)(I_y - 2I_y S_z)$	$-\sin((\omega_S - \pi J_{IS})t_1)(I_x - 2I_x S_z)$	o o
3B	$- \gamma_I/2\gamma_S g_4$	-y	x	$-0.5\sin((\omega_S - \pi J_{IS})t_1)(I_x - 2I_x S_z) + 0.5\cos((\omega_S - \pi J_{IS})t_1)(I_y - 2I_y S_z)$	$-\cos((\omega_S - \pi J_{IS})t_1)(I_y - 2I_y S_z)$	x o
4A	$ \gamma_I/2\gamma_S g_4$	-y	x	$0.5\sin((\omega_S + \pi J_{IS})t_1)(I_x + 2I_x S_z) + 0.5\cos((\omega_S + \pi J_{IS})t_1)(I_y + 2I_y S_z)$	$\sin((\omega_S + \pi J_{IS})t_1)(I_x + 2I_x S_z)$	o x
4B	$- \gamma_I/2\gamma_S g_4$	y	-x	$0.5\sin((\omega_S + \pi J_{IS})t_1)(I_x + 2I_x S_z) - 0.5\cos((\omega_S + \pi J_{IS})t_1)(I_y + 2I_y S_z)$	$\cos((\omega_S + \pi J_{IS})t_1)(I_y + 2I_y S_z)$	o o

¹ Sørensen, O. W.; Eich, G. W.; Levitt, M. H.; Bodenhausen, G.; Ernst, R. R. *Prog. NMR Spectrosc.* **1983**, 16, 163-192.

² Assuming the term $2S_x I_z$ is present at the beginning of t_1 .

³ Two free induction decays must be recorded per t_1 increment to obtain one subspectrum. Corresponding gradient and phase settings are indicated in rows labeled A and B.

⁴ By adding and subtracting the two data sets in column 5, the terms indicated in the table are obtained, A+B (normal text) A-B (boldface). These correspond to the real and imaginary parts of a hypercomplex data set recorded in the States manner, except the two signals are 90° out of phase in the acquisition dimension [States, D. I.; Haberkorn, R. A.; and Ruben, D. J. *J. Magn. Reson.* **1982**, 48, 286-292.]. Before applying a complex Fourier transform in the indirect dimension one of the two data sets must therefore be phaseshifted by 90° in the acquisition dimension.

⁵ This processing protocol is the standard processing scheme for experiments recorded with pulsed field gradients for coherence order selection. [Palmer, A. G.; Cavanagh, J.; Wright, P. E.; Rance M. *J. Magn. Reson.* **1991**, 93, 151-170. Kay, L. E.; Keifer, P.; Saarinen, T.; *J. Am. Chem. Soc.* **1992**, 114, 10663-10665.] In Bruker XWINNMR software, this corresponds to the “echo-antiecho” processing flag.