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Calculation of coherence pathway selection and cogwheel cycles

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Abstract

The selection of proper coherence pathways is a very important aspect of the design of NMR pulse sequences. This article describes a C++ program for the calculation of coherence pathway selection via phase cycles, including a module to calculate cogwheel cycles. Cogwheel phase cycles shorter than the original ones [M.H. Levitt et al., J. Magn. Reson. 155 (2002) 300] are derived and experimentally tested for the MQMAS experiment for 3/2 spins. Some other cogwheel cycles are derived for the MQNQMAS, the STMAS experiment, and a PFG diffusion pulse sequence. This program is publicly available through our website http://www.nyu.edu/projects/jerschow with additional documentation and examples.

Keywords: Coherence pathways; Cogwheel phase cycles; MQMAS; Pulsed field gradients; Quadrupolar nuclei; Diffusion measurements

1. Introduction

The selection of the appropriate coherence pathways is often an essential ingredient of solid- and liquid-state NMR pulse sequences [1–3]. The two main tools for achieving this are phase cycles and pulsed field gradients [4,5]. Other tools, such as the use of diffusion filters and flow-based coherence selection have been suggested [6]. Additionally, the use of echoes and nearly ideal π pulses can create a rather selective filtering [7]. The calculation of "ideal" phase cycles, i.e., the shortest ones, for a coherence selection problem has been done in some simple cases but a general solution seems elusive so far [8,9]. Furthermore, since one can apply pulsed field gradients and possibly other tools to aid the phase cycling in the selection process it seems difficult to devise a procedure of sufficient flexibility. Therefore the experimenter still needs to resort to empirical rules to set up phase cycles and pulsed field gradient sequences. The program presented here is very useful in this endeavor.

Recently, cogwheel phase cycling has been discovered [10], which can dramatically reduce the size of phase cycles in many cases. A number of impressive reductions have been shown (i.e., by a factor of 25 for a TOSS sequence). It is quite possible that cogwheel cycles are the most efficient phase cycles for a given selection problem. The program is intended to be rather flexible such as to accommodate most experimental situations, including heteronuclear experiments, and will be extended in the future to accommodate the calculation of the selection process imposed by pulsed field gradients, and possibly other means. The program presented here was equipped with a routine to calculate cogwheel phase cycles based on certain restrictions imposed by the user. As the tasks outlined above can lead to numerically quite demanding calculations this program provides the possibility, as its MATLAB predecessor [11], to restrict the calculation to subcycles with little effort. The program is written in C++ and we wish to call it CCCP++ (in reference to the earlier program CCCP—Complete Calculation of Coherence Pathways [11]). The current program is much more efficient and includes new features with regard to the calculation of the coherence pathway selection process by phase cycling. It is posted on the website: http://www.nyu.edu/projects/jerschow.

Several cogwheel cycles found by CCCP++ are discussed and shorter variants of the ones described in [10] are demonstrated experimentally.

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2. Phase cycling

The following treatment mainly follows [10,11] and includes some additional comments relevant to the program. A coherence pathway is written as $\mathbf{p} = (p_0, p_1, \ldots, p_n)$. The rf phases for a particular step with index m in the phase cycle are represented as a column vector, $\boldsymbol{\phi}^{(m)} = (\phi_1^{(m)}, \phi_2^{(m)}, \ldots, \phi_n^{(m)})^{\mathrm{T}}$, and the receiver phase is $\phi_{\mathrm{r}}^{(m)}$ (one may consider including in $\phi_{\mathrm{r}}^{(m)}$ a post-digitization phase shift [12,13]). The pulses may be performed on different channels for heteronuclear experiments. The difference coherence pathway is $\Delta\mathbf{p} = (p_1 - p_0, p_2 - p_1, \ldots, p_n - p_{n-1})$. The signal acquired in the receiver will have developed a phase due to the rf and receiver phases according to

$$\phi_{\mathrm{tot}}^{(m)} = -\Delta\mathbf{p} \cdot \boldsymbol{\phi}^{(m)} - \phi_{\mathrm{r}}^{(m)} \tag{1}$$

and the effective recorded signal is

$$s(\mathbf{p}) = \sum_{m=1}^{N} \exp(-\mathrm{i}\phi_{\mathrm{tot}}^{(m)}), \tag{2}$$

where N is the number of steps in the phase cycle. Choosing a proper coherence pathway assures that $s(\mathbf{p})$ is maximized (usually equal to N) for the desired pathways and is zero, or a small value for the undesired pathways. Until recently "nested" phase cycles have been used almost exclusively [2]. "Cogwheel phase cycles," on the other hand, have been found recently which require only a much reduced number of steps [10].

3. Cogwheel phase cycling

A set of so-called winding numbers is defined, $\boldsymbol{v} = (v_1, v_2, \ldots, v_n)^{\mathrm{T}}$, $v_i \in \{0, 1, 2, 3, \ldots\}$, which determine a given phase cycle, i.e., the mth step of the cycle is characterized by

$$\boldsymbol{\phi}^{(m)} = \frac{m2\pi}{N}\boldsymbol{v}, \tag{3}$$

where N is some positive integer that determines the number of steps in the phase cycle and m runs from zero to $N-1$. To insure the proper selection of a given desired coherence pathway, $\mathbf{p}^0$, the receiver phase for the mth step in the cycle needs to be set to

$$\phi_{\mathrm{r}}^{(m)} = -m\Delta\mathbf{p}^0 \cdot \boldsymbol{\phi}^{(m)}, \tag{4}$$

which corresponds to a receiver winding number $v_{\mathrm{r}} = \Delta\mathbf{p}^0 \cdot \boldsymbol{v}$. A cogwheel phase cycle is then uniquely determined by $(N; \boldsymbol{v}; v_{\mathrm{r}})$. Alternatively, a convenient definition might be $(N; \boldsymbol{v}; \mathbf{p}^0)$.

In order to find a set $(N; \boldsymbol{v}; v_{\mathrm{r}})$ it is necessary to insure that a minimum number of undesired coherence pathways is simultaneously selected by such a cycle. It is convenient to define a difference pathway $\mathbf{d} = \mathbf{p} - \mathbf{p}^0$ with the coherence differences $\Delta\mathbf{d} = (d_1 - d_0, d_2 - d_1, \ldots, d_N - d_{N-1})$. According to Eqs. (1), (3), and (4) a selected pathway $\mathbf{p}$ (with its corresponding $\Delta\mathbf{d}$) satisfies

$$\Delta\mathbf{d} \cdot \boldsymbol{v} \equiv 0 \pmod{N}. \tag{5}$$

Pathways, for which this equation is not satisfied will be canceled out, since

$$\sum_{m=0}^{N-1} \exp(-\mathrm{i}mk2\pi/N) = 0 \quad \text{for any } k \in 1, 2, \ldots, N-1. \tag{6}$$

It appears at this point that the winding numbers may be predicted only in very simple cases. In general a numerical search is necessary.

A simplification is possible in the common case where one of the elements of $\Delta\mathbf{p}$ is linearly dependent on the other elements for all considered coherence pathways. This happens, for example, when the initial coherence order is zero (equilibrium) and the last coherence order is minus one (detection) for all considered pathways. (The more general statement is that $p_n - p_0$ is the same number for all considered pathways.) Since

$$\Delta p_n = p_n - p_0 - \sum_{i=1}^{n-1} \Delta p_i \tag{7}$$

and

$$\Delta p_n^0 = p_n^0 - p_0^0 - \sum_{i=1}^{n-1} \Delta p_i^0 \tag{8}$$

one can rewrite Eq. (5) as

$$\Delta\mathbf{d} \cdot \Delta\boldsymbol{v} \equiv 0 \pmod{N}, \tag{9}$$

where

$$\Delta\boldsymbol{v} = (v_1 - v_n, v_2 - v_n, \ldots, v_{n-1} - v_n, 0). \tag{10}$$

One v_i may therefore be left out of consideration.

If additional constraints are available, additional winding numbers may be left out, as shown in an example below. These cases are particularly relevant for heteronuclear experiments and experiments employing pulsed field gradients.

4. Program

4.1. Input parameters

The program is supplied with a file specifying a number of parameters, some of which will be described for the ensuing discussion. A complete description can be found on the website.

For the calculation of the selected coherence pathways the following parameters may be supplied:

- A phase cycle is supplied in a common format, just as it would be input in an NMR pulse program.
- The pulses may act on different nuclear species.

- A special variable indicates which coherence orders shall be considered at each step in the pulse program, and for every nuclear species.
- An intensity threshold is supplied, below which the signal is treated as zero.

For the search for cogwheel cycles [10], the following parameters are used:

- The desired coherence pathway is specified, and can include separate pathways for each nuclear species.
- The maximum number of undesired pathways is specified that will be tolerated for an acceptable solution.
- The range of cogwheel cycle bases N to be searched is specified.
- It can be specified for which pulses no winding number need be searched. This is useful for speeding up the calculation in certain cases as discussed below. Again, this can be specified for each nuclear species separately.

4.2. Algorithm

The implementation of both the calculation of the pathway selection as well as the numerical search for cogwheel cycles was straightforward along the lines of the equations presented in the previous section. There are, however, some potential efficiency improvements that are in conflict with the overall goal of making the program flexible, incorporating the case of heteronuclei, and allowing the user to restrict the consideration to a subset of pathways.

For example, it may seem that the following procedure could speed up the calculation of coherence pathways. If, say, the phases $\phi_i^{(m)}$ for a given pulse i have a greatest common divisor $2\pi/k$ (with k a nonzero integer) the elements of Δp_i that need be considered are in $\{0, 1, \ldots, k-1\}$. This would be beneficial in many cases to cut down on the number of pathways to be considered. This procedure is, however, not very practical as the reconstruction of $\mathbf{p}$ from $\Delta\mathbf{p}$ is a computationally inefficient procedure because of the additional uncertainty in the definitions of its elements (mod k). This procedure becomes even less attractive when one considers heteronuclear spin systems, or when certain pathways are to be neglected through input by the user. Finally, cogwheel phase cycles almost always have N much larger than the maximum considered coherence order and the restriction of the coherence order jump to a region $0, 1, \ldots, N-1$ represents no advantage at all in this case.

Since the actual calculation of the signal intensities according to Eq. (2) is not a very costly procedure (the necessary sin and cos factors can be prestored), it seems reasonable to simply run a loop through all possible coherence pathways $\mathbf{p}$, considering the restrictions imposed by the user.

The following observation may be useful in searching for new cogwheel cycles. It was found in all our numerical searches so far that if for a given N-step cycle an appropriate $\boldsymbol{v}$ is found, other $(N+1)$- and $(N+2)$-step cycles could be found. Therefore, in scanning the numbers N it is useful to search in large increments and gradually narrow them down. No rigorous proof for this has been found so far, so it cannot be guaranteed that the cycles found will also represent the minimal cogwheel cycles. A crude estimation of the minimum N cogwheel cycle may be obtained by $N \geqslant \prod_{i=1}^{n}(2p_{\max}^{(i)}+1)$, where n is the number of pulses, and $p_{\max}^{(i)}$ is the maximum coherence order at step i in the pulse sequence. In this particular case, it was assumed that p_0 is the same value for all considered pathways. This consideration is motivated by the fact that $\boldsymbol{v}$ can always be chosen to be

$$\boldsymbol{v} = \left(1, [2p_{\max}^{(1)}+1], \ldots, \prod_{i=1}^{n-1}[2p_{\max}^{(i)}+1]\right)^{\mathrm{T}} \quad (11)$$

to make $\sum_i \Delta d_i v_i$ have distinct values for all Δd_i except the trivial case $\Delta\mathbf{d} = 0$, which indicates the desired coherence pathway. It is, however, quite likely that much tighter bounds on N can be found, especially in cases where not all coherence orders ranging from $-p_{\max}^{(i)}$ to $+p_{\max}^{(i)}$ are allowed.

5. Experimental

A well-crystallized sample of $RbNO_3$ was selected for the experimental investigation. The fine powdered sample was packed in a 4-mm MAS rotor. All the experiments were performed on a Bruker AV 400 MHz NMR spectrometer equipped with a 9.4-T wide bore ultrashielded magnet. ^{87}Rb MQMAS spectra were recorded at a Larmor frequency of 130.927 MHz. The FAM-RIACT-FAM MQMAS pulse sequence [14,15] was used (Fig. 1).

The spinning frequency was 8 kHz. The rf powers used for the strong and soft pulses were 27.7 and 4.3 kHz. The RIACT pulse was applied for a duration of 31.25 μs. The FAM interval consisted of $n = 4$ cycles of pulse-delay-pulse-delay, with each element lasting 1 μs and a π phase difference between consecutive pulses. A total of $256 t_1$ and $1024 t_2$ data points were acquired and covered a spectral window of 2812.5 Hz × 50 000 Hz. The recycle delay was 1 s.

6. Results and discussion

Levitt and coworkers have found the smallest possible cogwheel cycle for a MQMAS experiment for $I = 3/2$ spins [10], which selects only the desired

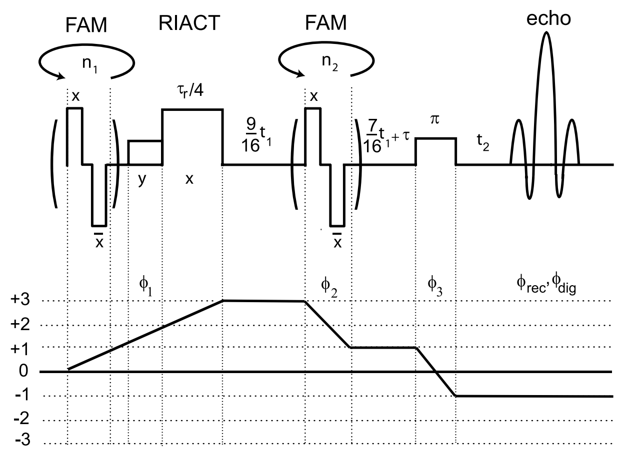

Fig. 1. FAM-RIACT-FAM MQMAS pulse sequence. The pulse lengths were 1, 1, 9, 31.25, 1, 1, and 48 μs for all pulses in sequence. The pulses drawn with lower amplitude indicate selective pulses applied to the central transition. The first FAM sequence, the first soft pulse and the RIACT pulse were phase cycled together.

coherence pathway (Fig. 1) under the assumption that only −1 coherence is detected (perfect quadrature detection). Here we examine, how one can derive other cycles using this program by specifying quite reasonable restrictions on the coherence pathways. The cogwheel cycles are indicated in the notation $\mathrm{COGN}(\nu_1, \nu_2, \nu_3; \nu_r)$ [10].

- $\mathrm{COG29}(9, 11, 2; 28)$. This cycle selects only the desired pathway even when the detection coherence order may be −1, 0, or +1 (imperfect quadrature detector). The experiment is shown in Fig. 2a

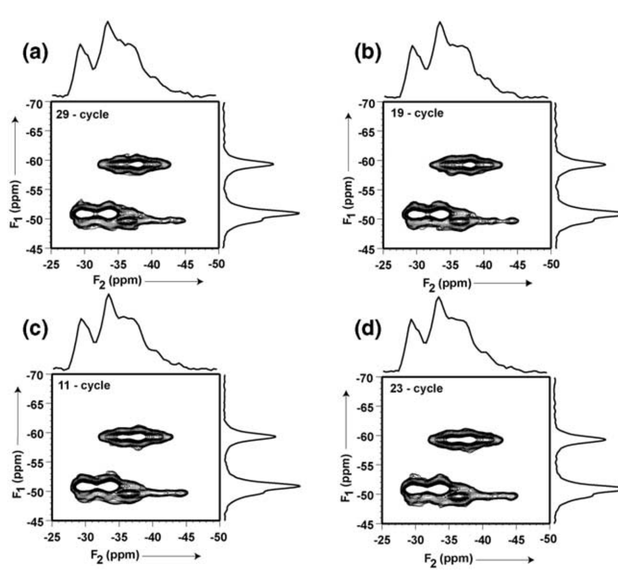

Fig. 2. ^{87}Rb MQMAS spectra taken from a solid $RbNO_3$ sample using the pulse sequence of Fig. 1 and the cogwheel phase cycles (a) $\mathrm{COG29}(9, 11, 2; 28)$, (b) $\mathrm{COG19}(3, 8, 1; 9)$, (c) $\mathrm{COG11}(3, 1, 0; 4)$, and (d) $\mathrm{COG23}(3, 0, 22; 12)$. In order to make the total number of scans similar (a) 58, (b) 57, (c) 66, and (d) 69 scans were acquired for each transient.

- $\mathrm{COG19}(3, 8, 1; 9)$. This cycle also considers an imperfect quadrature detector, but restricts the pathways to odd and zero coherence orders. The experiment is shown in Fig. 2b.
- $\mathrm{COG11}(3, 1, 0; 4)$. Here, a perfect quadrature detector is assumed, and only odd coherence orders plus zero order are considered. The experiment is shown in Fig. 2c.

For comparison, an experiment was also performed with one of the 23-step cogwheel cycles [10], $\mathrm{COG23}(3, 0, 22; 12)$, a spectrum of which is shown in Fig. 2d. For half-integer quadrupolar spins it appears quite reasonable to disregard pathways with even coherence orders (except zero order), since those pertain to satellite transitions. While single-quantum coherences of satellite transitions are now detected on a routine basis in STMAS experiments [16,17], they still have comparatively weak intensities when the magic angle is not set extremely accurately [18–20]. It is expected that higher quantum satellite transitions will produce quite weak signal intensities, and could be attenuated further by deliberately offsetting the rotor axis from the magic angle by a small amount (up to 0.05°). Such a small offset will have virtually no effect on the appearance of the signal coming from odd coherence orders.

Apart from a change in the signal-to-noise ratios related to the differences in the numbers of accumulated transients, no disparities are seen in the spectra. It can be assumed that the 11-step cycle performs just as well as the 23-step cycle in this case.

For a 5Q3QMAS [21] experiment (Fig. 3a), for example, the following cogwheel cycles may be used: $\mathrm{COG201}(157, 142, 3, 0; 108)$ considering all possible pathways and a perfect quadrature detector, COG55 $(33, 30, 1, 0; 7)$ when only odd coherence orders plus zero order are considered, and $\mathrm{COG29}(3, 1, 0, 0; 16)$ when in addition the last two coherence orders are restricted to $(1, -1)$. The last requirement may seem too stringent but it is easily realizable in practice by choosing a relatively long echo delay.

For the $I = 3/2$ SCAM-STMAS experiment with a split-t_1 delay and compensation for magic-angle offset effects [19,20] (Fig. 3b) an appropriate cycle would be $\mathrm{COG87}(75, 9, 1, 0; 12)$ considering a perfect quadrature detector and $\mathrm{COG21}(9, 1, 0, 0; 12)$ if a perfect echo can be assumed at the end. The corresponding nested phase cycles would be of size 125 and 25, respectively, for a 3/2 spin. The gains may be greater for higher spins.

Another experiment where cogwheel cycles may prove to be very useful is the diffusion experiment employing bipolar field gradients and a longitudinal eddy current delay (Fig. 3c) [22]. The phase cycles used previously were based on a compromise between size and selectivity. A good way to find a useful cogwheel cycle is to consider the two spoiler gradients to be orthogonal to the diffusion gradients and to each other. In this case

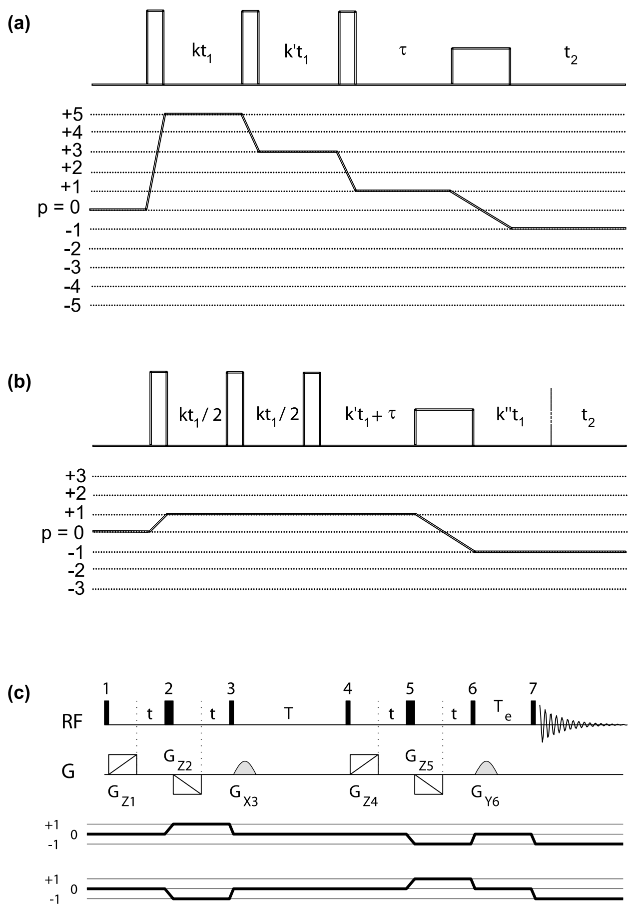

Fig. 3. (a) 5Q3QMAS sequence, (b) SCAM-STMAS sequence. The symbols used have their standard meanings. (c) PFG stimulated echo pulse sequence for measuring diffusion coefficients, employing bipolar gradients [22] and a longitudinal eddy current delay. All pulses are 90° pulses except pulses 2 and 5, which are 180° pulses. The gradients G_{Z1}, G_{Z2}, G_{Z4}, and G_{Z5} (also termed "diffusion gradients") are ramped up during a diffusion experiment. The coherence selection afforded by those should not be taken into account, since the experiment should provide consistent data down to very weak Z gradients. The gradients G_{X3} and G_{Y6} are spoiler gradients to remove any coherence of order other than zero and are orthogonal to each other and to the diffusion gradients.

one may consider the coherence orders after the third and sixth pulses to be restricted to zero. Then $\Delta p_1 + \Delta p_2 + \Delta p_3 = 0$, and $\Delta p_4 + \Delta p_5 + \Delta p_6 = 0$, and one can set v_1 and v_4 to zero in the search, in addition, if perfect quadrature detection is assumed (and there are few reasons to do otherwise with modern hardware), $v_7 = 0$. In this case the computational effort to find a proper cycle is minimized. If the maximum coherence order is two (for a two-spin system), a cycle that selects only the two desired pathways $(0, -1, 1, 0, 1, -1, 0, -1)$ and $(0, 1, -1, 0, -1, 1, 0, -1)$ is $\mathrm{COG80}(0, 58, 18, 0, 3, 1; 13)$. If the diffusion experiment is run on a one-spin system (e.g., water) the cycle $\mathrm{COG8}(0, 7, 0, 0, 1, 0; 4)$ is found. By contrast, the shortest conventional cycle to achieve this would have $2 \times 4 \times 4 \times 4 = 128$ and $2 \times 4 \times 3 \times 4 = 96$ steps, respectively (in the latter case the second and the fourth cycles may not be reduced to three, for this would make it impossible to retain both pathways). It is expected that useful cycles can be found for the convection-compensated siblings of this experiment [23].

Further experiments where the procedure of finding short cogwheel phase cycles might even be more impressive include MQNQMAS for higher spins, the QCPMG experiment [24,25], and the QPASS experiment [26].

7. Compatibility and availability

The program was written in ANSI C++ using the Standard Template Library. It is expected to compile without difficulties (using the supplied Makefile) on any GNU g++ compatible compiler of version 2.95 or higher. Some lower versions probably would work also, as well as older compilers as long as they are ANSI compliant. It has been compiled on Linux (Mandrake 8.2, i586), and SGI (Irix 6.5, mips R12000). The parsing module was created using flex++ version 2.5.1 and 2.5.4, it is possible that these versions or later are required, although this could not be verified (flex++ is available under the GNU license). The program itself including all source code is given away under the GNU license, and is available for download at http://www.nyu.edu/projects/jerschow.

8. Conclusion

A C++ program is presented for the calculation of the coherence pathway selection process by phase cycling. A module is included to calculate cogwheel cycles. Issues related to efficiency have been discussed. Some improvements to the program are planned, including the calculation of attenuation by pulsed field gradients, and the analysis of imperfect 180 in the selection process [7].

Some new cogwheel cycles are presented for the MQMAS, the MQNQMAS, and the SCAM-STMAS experiments. Experiments demonstrate the performance of some of these cycles for MQMAS. A cogwheel cycle is also presented for the stimulated echo diffusion experiment employing bipolar gradients.

Finally, the program may be useful for interfacing with NMR simulation software, where prior knowledge of the possible coherence pathways may speed up the calculations significantly.

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