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In this study, the performance of a virtual Frisch-grid cadmium zinc telluride (CZT) detector was estimated for the analysis of the 14 MeV neutron-activation prompt γ-rays using the Monte Carlo simulation. The size of the CZT single crystal was 6 × 6 × 15 mm3, which was designed based on an actual model develop at the Brookhaven National Laboratory (BNL). The amount of carbon and oxygen in TNT and cocaine samples were measured by detecting the prompt γ-rays after neutron inelastic scatterings, and the carbon-to-oxygen peak ratio of the target materials was used to identify the suspicious materials. The prompt γ-rays peaks could be efficiently distinguished in the energy spectrum when the sensitive nonlinear iterative peak (SNIP) clipping algorithm, including the subtraction of background counts, was applied to the spectrum. The energy spectrum modified using the SNIP algorithm showed higher performance than the original energy spectrum for the analysis of the carbon-to-oxygen ratio. The results of the simulation proved the effectiveness of the CZT detector to detect and analyze the prompt γ-rays in the prompt γ-ray neutron activation analysis (PGNAA).

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This paper is about the performance estimation of virtual Frisch-grid CdZnTe detector for prompt γ-ray induced by 14 MeV neutron. The carbon to oxygen element ratios of the explosive and narcotic materials were determined from the simulated prompt γ-ray yields. The results of the simulation for C/O ratios showed similar trends as the theoretical values. The energy spectrum obtained using the SNIP algorithm demonstrated superior performance than the original energy spectrum for the C/O ratios in TNT and cocaine samples.

Performance estimation of virtual Frisch-grid CdZnTe detector for prompt γ-ray induced by 14 MeV neutron: Monte Carlo simulation study

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Abstract— In this study, the performance of a virtual Frisch-grid cadmium zinc telluride (CZT) detector was estimated for the analysis of the 14 MeV neutron-activation prompt γ-rays using the Monte Carlo simulation. The size of the CZT single crystal was 6 × 6 × 15 mm^3, which was designed based on an actual model develop at the Brookhaven National Laboratory (BNL). The amount of carbon and oxygen in TNT and cocaine samples were measured by detecting the prompt γ-rays after neutron inelastic scatterings, and the carbon-to-oxygen peak ratio of the target materials was used to identify the suspicious materials. The prompt γ-rays peaks could be efficiently distinguished in the energy spectrum when the sensitive nonlinear iterative peak (SNIP) clipping algorithm, including the subtraction of background counts, was applied to the spectrum. The energy spectrum modified using the SNIP algorithm showed higher performance than the original energy spectrum for the analysis of the carbon-to-oxygen ratio. The results of the simulation proved the effectiveness of the CZT detector to detect and analyze the prompt γ-rays in the prompt γ-ray neutron activation analysis (PGNAA).

Keywords— Virtual Frisch-grid cadmium zinc telluride (CZT), Monte Carlo simulation, sensitive nonlinear iterative peak clipping algorithm (SNIP), prompt γ-ray neutron activation analysis (PGNAA).

1. Introduction

If an atomic nucleus of target materials is exposed to high-energy neutrons, the neutron-induced prompt γ-ray with a characteristic energy is emitted from an unstable nucleus. Even if the elements of the target materials are not previously identified, it is possible to identify these elements based on the differences in the neutron-induced prompt γ-ray peaks. This principle is applied to the prompt γ-ray neutron activation analysis (PGNAA) (Engesser and Thompson, 1967; Strellis and Gozani, 2005; Perot et al., 2008; Jun et al., 2011). Because the PGNAA method is useful for the analysis of a suspicious material, it can be applied to detect the illegal explosives and drugs at an airport or a harbor (Shea et al., 1990; Miller, 1994; Pesente at al., 2004). In addition, the composition of the target material can be estimated without using a chemical component test or destructive techniques (Paul and Lindstrom, 2000; Nunes et al., 2002; Nasrabadi et al., 2011). The differences in the prompt γ-ray peaks observed in an energy spectrum depend on the energy resolution of a radiation detector. Therefore, high-purity germanium (HPGe) semiconductor detectors that have high-energy resolution are utilized to conduct PGNAA (Seabury et al., 2007; Nicol et al., 2016). However, their portability is limited due to the need for cooling devices at room temperature.

The lanthanum bromide ($LaBr_3$:Ce) scintillation detector, which has a higher energy resolution than conventional scintillators, has been employed in PGNAA without the need for cooling devices. The results of the detection of prompt γ-rays in bulk samples with C, O, and H concentrations demonstrated the superiority of the $LaBr_3$ detector (Naqvi et al., 2012) and the experimental data were in good agreement with the theoretical values (Naqvi et al., 2013).

Cadmium zinc telluride (CZT) detectors have been developed as an alternative for the room temperature operation with good energy resolution. To overcome the low mobility of holes in a material and its non-uniformity, the specially designed CZT detectors, such as the co-planar grid (Luke and Eissler, 1996), small pixel structure (He et al., 1999; Zhang et al., 2004), and virtual Frisch-grid (McGregor et al., 1998; McNeil et al., 2004; Harrison et al., 2007), were developed to measure the radiation energy. Particularly, the electrode structure of the virtual Frisch-grid CZT detectors that use small number of read-out channels per detector element was simpler than the multi-pixel CZT detectors (Bolotnikov et al., 2012, 2015). Hence, these devices are ideal to build blocks for assembling arrays because the size of the detector is not limited by the crystal size (Bolotnikov et al., 2015; Lee et al., 2016).

Our research that uses the Monte Carlo n-particle extended (MCNPX) code is focused on the performance estimation of the detection system to monitor suspicious materials in homeland security. In this study, we simulated the prompt γ-rays, emitted by the elements of the target materials during irradiation with a 14 MeV neutron beam, using a virtual Frisch-grid CZT detector. The energy resolution of the virtual Frisch-grid CZT detector, based on an actual model developed at the Brookhaven National Laboratory (BNL), was used to analyze and distinguish the prompt γ-rays peaks. Subsequently, a sensitive nonlinear iterative peak (SNIP) clipping algorithm, including the subtraction of the background counts, was applied to obtain the energy spectrum rapidly and accurately, and the results of the energy spectrum were compared to those of the original energy spectrum. Finally, the carbon-to-oxygen (C/O) ratio was calculated using the effective counts of the characteristic γ-ray peak in the energy spectrum for the identification of the explosives and narcotic.

2. Design and methods

Fig. 1 shows the actual model of the virtual Frisch-gird CZT single crystal that was developed at the Brookhaven National Laboratory (BNL) (Bolotnikov et al., 2012, 2015). The detector has a volume of 6 × 6 × 15 mm^3. In the PGNAA simulation, the Monte Carlo N-Particle eXtended (MCNPX) code was used to estimate the performance of the virtual Frisch-grid CZT detector, which was designed based on an actual model.

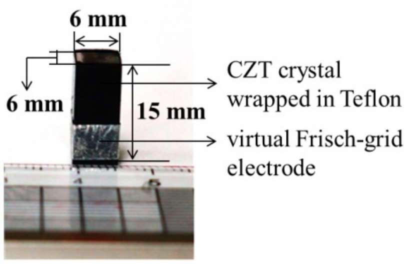

Fig. 1. Photograph of the virtual Frisch-grid CZT single detector.

The schematic diagram of the Monte Carlo simulation study is shown in Fig. 2. The geometrical structure of the detection system was referred from other studies (Naqvi et al., 2012, 2013). When a 14 MeV neutron beam is exposed to an unknown target nucleus, the prompt γ-rays, which have characteristic energy peaks of the target nucleus, are detected by the detection system. Hence, the elements of the target material can be identified by analyzing the prompt γ-ray peaks (Table 1). In particular, illegal materials such as explosives and narcotic can be distinguished based on their characteristic C/O element ratio. Hence, TNT and cocaine were chosen for our research. Table 2 shows the elemental compositions of the target materials. The distance between neutron source and the center of the target was set to 100 cm, and the distance between the CZT detector and center of the spherical target was set to 7 cm. The diameter of the target was set to 2 cm. The orthogonal positioning prevented the detector from interacting with the neutron source. Moreover, the CZT detector was shielded from the incident 14 MeV neutron beam and the neutron-induced γ-ray background through paraffin, tungsten, and lead shielding. The target materials were irradiated with a neutron flux of 2.0 × 10^{10} n/cm^2·s, as reported in a previous study (Jakhar et al., 2008). The exposure time was 1.0 s.

Table1
Selected elements and relevant nuclear information (Womble et al., 1995; Im and Song., 2009).

Elements	Reactions	Cross section (mb) at 14 MeV	Prompt γ-ray energy (MeV)
C	^{6}C(n, n′, γ)^{6}C	200	4.44
O	^{8}O(n, n′, γ)^{8}O	750	6.13

Table2
Elemental compositions of TNT and cocaine (Strellis and Gozani, 2005).

Material	Density (g/cm^3)	%H	%C	%N	%O	Elemental ratio (C/O)
TNT ($C_3H_5O_6N_3$)	1.63	2.2	37	18.5	42.3	0.9
Cocaine ($C_{17}H_{21}NO_4$)	0.84	6.9	67.3	4.6	21.1	3.2

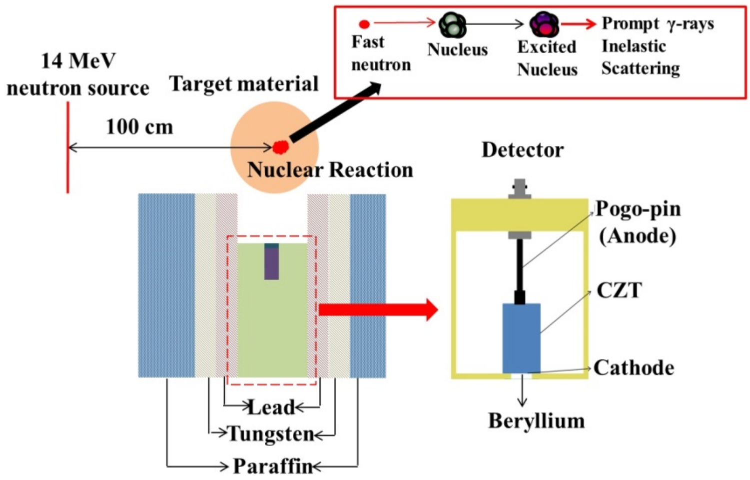

Fig. 2. Schematic diagram of simulation setup of prompt γ-ray neutron activation analysis (PGNAA).

For a more realistic performance evaluation of the virtual Frisch-grid CZT detector obtained by performing the MCNPX simulation, it is necessary to consider the energy resolution by applying the Gaussian energy broadening (GEB) parameters. Using a fitting function shown in Eq. (1), the values of coefficients *a*, *b*, and *c*, which will be used as inputs to the MCNPX code, were calculated (Pelowitz., 2005; Salgado et al., 2012). The parameters specify the full width at half maximum (FWHM) of the observed energy broadening in a detector.

$$\mathrm{FWHM} = a + b\sqrt{E + cE^2} \tag{1}$$

, where E is the incident γ-ray energy (MeV). The units of a, b, and c are MeV, MeV$^{1/2}$, and 1/MeV, respectively. The FWHM of the virtual Frisch-gird CZT single detector was determined based on the energy resolution measured in experiments. Table 3 shows the specifications of the virtual Frisch-gird CZT single detector (Bolotnikov et al., 2012, 2015) and GEB values of the MCNPX simulation.

Table 3
The specification of the virtual Frisch-gird CZT single detector for the MCNPX simulation.

Density (g/cm^3)	Energy resolution at 511 keV (%)	Energy resolution at 662 keV (%)	GEB value (a)	GEB value (b)
5.60	2.0	1.0	0.0360	-0.0360

For the selection of effective counts, a ± 0.45% energy window was employed around the photoelectric peak in the energy spectrum of each element. Although the measured counts of each characteristic photoelectric peak for the prompt γ-ray are related to the compositions of the target materials, the ratio of the photoelectric peak counts of each element does not directly reflect the composition ratio of the target materials. Hence, various factors for different energies of prompt γ-rays were considered to estimate the composition ratio of the target materials, as shown in the Eq. 2 (Carasco et al., 2007).

$$\frac{R_A}{R_B} = \frac{\sigma_B(E_n)B_B(E_r)\varepsilon_B(E_r)}{\sigma_A(E_n)B_A(E_r)\varepsilon_A(E_r)} \times \frac{C_A(E_r)}{C_B(E_r)} \tag{2}$$

, where $\sigma(E_n)$ is the neutron absorption cross-section for neutron energy E_n (14 MeV) (Womble et al., 1995), $B(E_r)$ is the branching ratio of the prompt γ-ray with energy E_r, $\varepsilon(E_r)$ is the detection efficiency of the CZT detector at E_r, and $C(E_r)$ is the counts within the photoelectric peak at energy E_r.

To rapidly and easily identify the elemental compositions of the target materials, the SNIP algorithm was applied to obtain the energy spectrum (Ryan et al., 1988; Hampton et al., 1994). This method that subtracts the baseline from the original energy spectrum can extract γ-ray peaks without background noise. Previous studies derived SNIP algorithm for proton-induced X-ray and γ-ray spectroscopies (Ryan et al., 1988; Hampton et al., 1994). The *C* language of the SNIP algorithm was derived by Morháč et al. (1997). Hence, the energy spectrum obtained using the SNIP algorithm demonstrated the minimum background noise and highlighted the prompt γ-ray peaks.

3. Results and discussion

To estimate the real performance of the virtual Frisch-grid CZT detector obtained by performing the MCNPX simulation, the energy spectra measured during the experiment and calculated during the simulation were compared to each other. Fig. 3 shows the comparison between the experimental and simulated energy spectra using the MCNPX code. There was a slight distortion around the photoelectric peak in the experimental energy spectrum due to the tail effect in the CZT semiconductor detector, which was caused by the slow charge collection and relatively small mobility lifetime of the holes (Bolotnikov et al., 2012, 2015). However, the trends of the measured energy spectrum and calculated energy spectrum were similar to each other. These results demonstrated the feasibility of estimating the real performance of the virtual Frisch-grid CZT detector through the results obtained using the MCNPX code in the prompt γ-ray activation analysis.

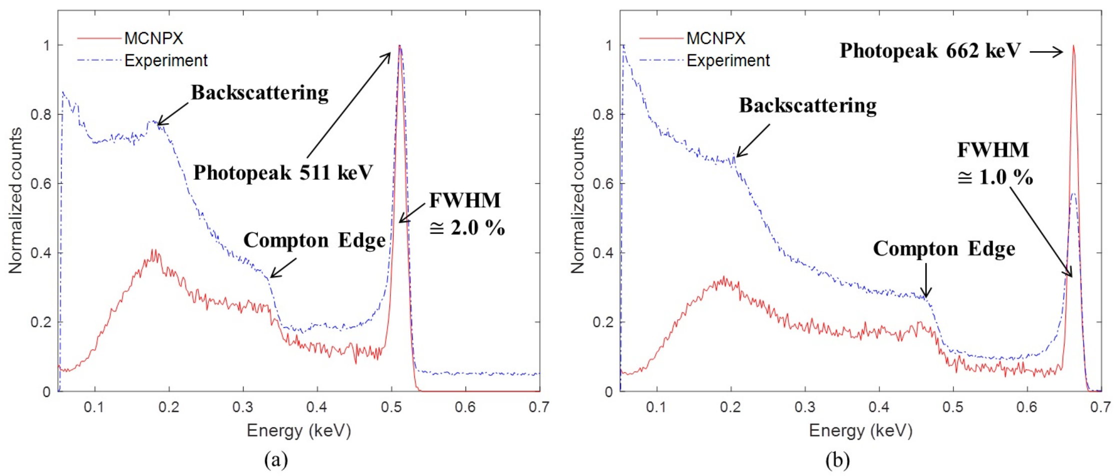

Fig. 3. Comparison between experimental and simulated pulse height distributions to point sources: (a) 511 keV, (b) 662 keV.

To estimate the performance of the prompt γ-ray yields and the minimum detection level (MDL) of the concentration of elements, the simulated energy spectrum of the virtual Frisch-grid CZT detector for carbon and oxygen peaks in an artificial sample was analyzed. The artificial sample consisted of carbon and oxygen of diameter 2 cm (density = 2.0 g/cm^3). The composition of the each elemental ratio was gradually changed to verify the prompt γ-ray yields of carbon and oxygen. Figs. 4(a) and 5(a) show the γ-ray yields as the function of carbon and oxygen concentrations in an artificial sample with CZT detector. As shown in Figs. 4(a) and 5(a), the solid line (blue) and dotted line (red) represent the γ-ray yields in the original energy spectrum and energy spectrum, respectively, with the rejection of the background noise using the SNIP algorithm. The γ-ray yields of each element in the target material increase as the concentration of element increases. As the iterations of the SNIP algorithm increased, the baseline of the energy spectrum decreased, and the noise that should be removed was not included in the baseline. Hence, the 6th iteration was chosen in which the result showed the energy spectrum without a significant noise peak. The MDL, which is calculated based on the "Currie equation", is defined as the limit to which the measured counts and the background counts can be discriminated. It was calculated as

$$\mathrm{MDL} = 4.65\sqrt{N_B} + 2.71 \tag{3}$$

, where N_B is the background counts under the peak of each element in the energy spectrum. Figs. 4(b) and 5(b) show the MDL as the function of the concentration of each element in an artificial sample. The results demonstrate that a virtual Frisch-grid CZT detector is appropriate to measure main elements such as C and O in explosives and narcotic in the prompt γ-ray activation analysis.

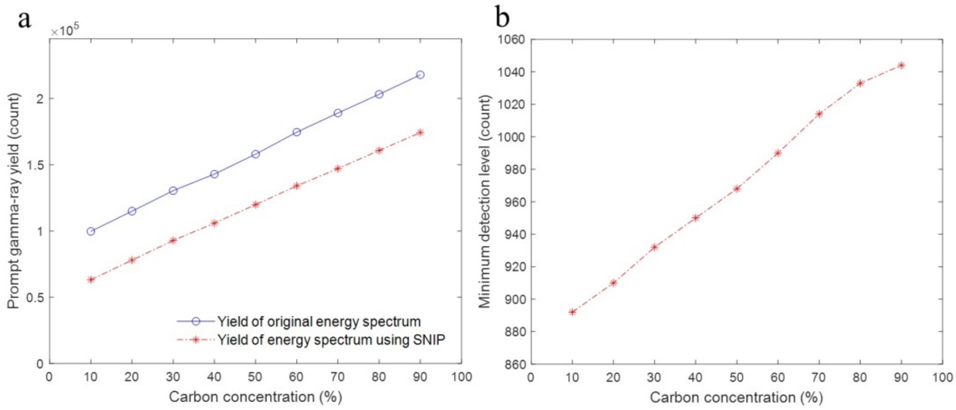

Fig. 4. Estimated performance after neutron inelastic scattering using MCNPX code for carbon element. (a) Prompt γ-ray yield, and (b) MDL.

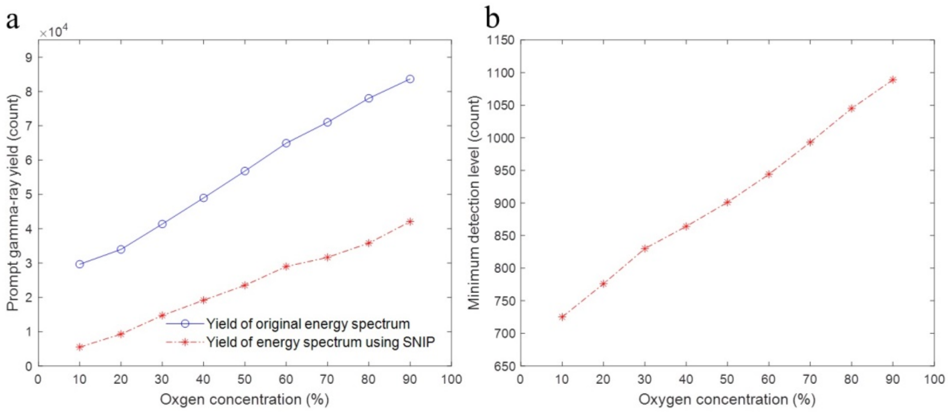

Fig. 5. Estimated performance after neutron inelastic scattering using MCNPX code for oxygen element. (a) Prompt γ-ray yield, and (b) MDL.

Fig. 6 shows the prompt γ-ray spectra of the TNT and cocaine samples. All elements observed in the analyzed explosives and narcotic were clearly identified using the data obtained by the virtual Frisch-grid CZT detector. The TNT and cocaine samples could be distinguished based on their characteristic C/O elemental ratios. TNT exhibited a small C/O ratio, whereas cocaine exhibited a high C/O ratio. Based on the counts of the energy spectrum of each element using the SNIP algorithm, various performances of the detection system were estimated.

The ratio of C/O of the theoretical value and the estimation of the simulation results were similar to each other. Moreover, the result obtained using the SNIP algorithm showed less deviation from the theoretical values than that obtained without the SNIP algorithm. The energy resolutions and the minimum detection level (MDL) of the prompt γ-ray peaks using the simulation are shown in Table. 4. Due to the limitation of the thickness of the virtual CZT detector, single and double escape peaks from carbon and oxygen were detected significantly. However, these peaks were completely different from the major elements of the target materials used to determine the explosives and narcotic.

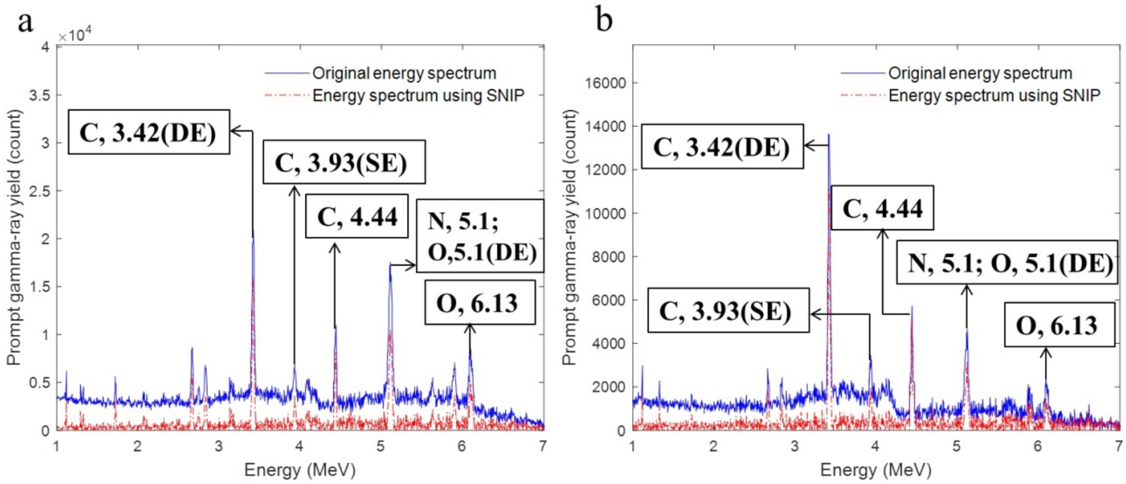

Fig. 6. Estimated prompt γ-ray energy spectrum after neutron inelastic scattering using MCNPX code. (a) TNT, and (b) cocaine. SE and DE refer to the single escape peak and the double escape peak, respectively.

Table 4
Estimation of the performance for the TNT and cocaine samples.

Material	Theoretical value (C/O)	Simulation result		Difference (%)		Energy resolution (%, with SNIP)		Minimum detection level (MDL)	
		Without SNIP	With SNIP	Without SNIP	With SNIP	4.44 MeV	6.13 MeV	4.4 MeV	6.13 MeV
TNT	0.9	0.937	0.912	3.9	1.3	0.45	0.48	556	899
Cocaine	3.2	3.36	3.28	4.7	2.4	0.45	0.32	471	389

4. Conclusions

Based on the prompt γ-rays induced by 14 MeV neutron from carbon and oxygen in TNT and cocaine samples, PGNAA using Monte Carlo simulation was performed to estimate the performance of the virtual Frisch-grid CZT detector. The carbon to oxygen element ratios of the explosive and narcotic materials were determined from the simulated prompt γ-ray yields. As expected, the explosive material showed smaller C/O ratios, whereas the narcotics material showed a high C/O ratios. The results of the simulation for C/O ratios showed similar trends as the theoretical values. In particular, the energy spectrum obtained using the SNIP algorithm demonstrated superior performance than the original energy spectrum for the C/O ratios in TNT and cocaine samples. The performance of the simulation results demonstrated that the virtual Frisch-grid CZT detector is suitable for the PGNAA application.

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