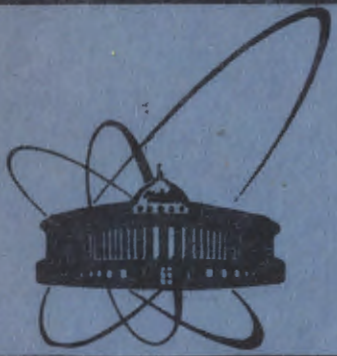

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ELECTRIC FIELD GRADIENTS AT Gd IN GADOLINIUM AND RARE EARTH TRIFLUORIDE SINGLE CRYSTALS

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1. INTRODUCTION

In the last few decades experimental and theoretical studies of crystal field effects in crystals containing rare earth ions have become of considerable interest [1]. The crystalline electric field (CEF) determines mainly the magnetic, transport, thermal, and optical properties of these substances. Very powerful methods for studying the CEF are the spectroscopic ones, for example: optical absorption for isolators, magnetic and γ-resonances, and neutron scattering for metallic and isolating samples.

The electric field gradient (EFG) at the site of a nucleus as the spatial derivation of the CEF is produced by an asymmetric distribution of charges in the lattice space and within the ion itself. The interaction of the EFG with the nuclear quadrupole moment is the electric part of the hyperfine interactions, and it causes a perturbation of the angular correlation (PAC) of γ-rays from a cascade transition of an excited nucleus [2]. Because of the absence of the orbital angular momentum of the 4f-electrons in their ground state the Gd^{3+} ion seems to be the most appropriate as a probe from rare earth ion for applying in the PAC technique. The half-filled 4f-shell in the Gd^{3+} ion has spheric symmetry and does not give any contribution to the EFG at the nuclear site. The EFG at such a probe nucleus in a noncubic metallic lattice is usually written as

$$V = V_{latt} \ (1 - \gamma_\infty) + V_{el} \ , \qquad (1)$$

where the lattice part V_{latt} comes from the ions in the lattice and can be calculated by lattice sum methods. The Sternheimer antishielding factor γ_∞ takes into account the shielding effects of the closed electron shells in the ion. For the Gd^{3+} ion it has been obtained $\gamma_\infty = -75$ [3]. The electronic part in eq. (1) includes the contribution from the conduction electrons to the EFG and is difficult to estimate theoretically. However, many of the available data seem to obey a simple empirical formula for the relation between the lattice and electronic parts of the EFG [4]:

$$V_{el} = -K V_{latt} (1 - \gamma_\infty), \qquad (2)$$

where K is about three.

The PAC method allows one to determine the components of the EFG tensor in its principal axes system: V_{zz}, $\eta = (V_{xx} - V_{yy})/V_{zz}$. The magnitude of the PAC depends upon these EFG parameters and on the life time τ and the quadrupole moment Q of the intermediate state of the nucleus. In the case of axial symmetry of the EFG tensor ($\eta = 0$), the essential parameter measured by the PAC method remains the frequency of "quadrupole precession"

$$\omega_0 = p \frac{eQV_{zz}}{4hI(2I-1)}, \qquad (3)$$

where p = 3,9,15 for integer nuclear spins I.

In this paper the results of EFG measurements on ^{154}Gd nuclei as probes in monocrystals of Gd and RF_3 (R = La, Ce, Pr, Nd, Sm, Eu, Gd) using the method of the integral perturbation of angular correlation (IPAC) are reported. The experimental data were compared with the values of the EFG from a point charge model calculation and with values derived from CEF parameters obtained by measurements of the electron paramagnetic resonance (EPR)[5-7], the nuclear quadrupole resonance[8,9], and the optical absorption in rare earth fluorides[10,11].

2. EXPERIMENT AND METHOD

The most of the investigated single crystals were grown by the "Bridgman-Stockbarger" method[12]. The GdF_3 single crystals were obtained from the firm "Alfa-Ventron" (USA).

For the IPAC measurement the source nuclei ^{154}Eu were produced by the reaction $^{153}Eu(n,p)\,^{154}Eu$, separated by an electro-magnetic mass separator, and than implanted into the samples, using an accelerating potential of 70 kV. The IPAC measurements were performed at room temperature by the spectrometers described in refs.[13,14]. In order to get a minimal statistical error we have used four (γ-γ)-cascades (247-123), (873-123), (1005-123) and (1274-123) keV, by averaging the resulting EFG parameters obtained for every of these cascades.

The axial symmetry of the lattice sites in Gd allows one to use the program QUDIM[15] for treating the experimental data, which yields ω_0, and V_{zz} was obtained by eq.(3). The EFG parameters for the fluorides, however, were determined by the method including the diagonalization of the hyperfine interaction Hamiltonian described in ref.[16,17].

3. RESULTS AND DISCUSSION

3.1. EFG in Gadolinium

Several authors have investigated the EFG in gadolinium by the methods of Mössbauer spectroscopy (ME)[18-21] and of angular distribution after the Coulomb excitation (CE)[22,23]. In Table 1 it is shown, that the values of the EFG in Gd obtained by these methods are rather different.

Table 1

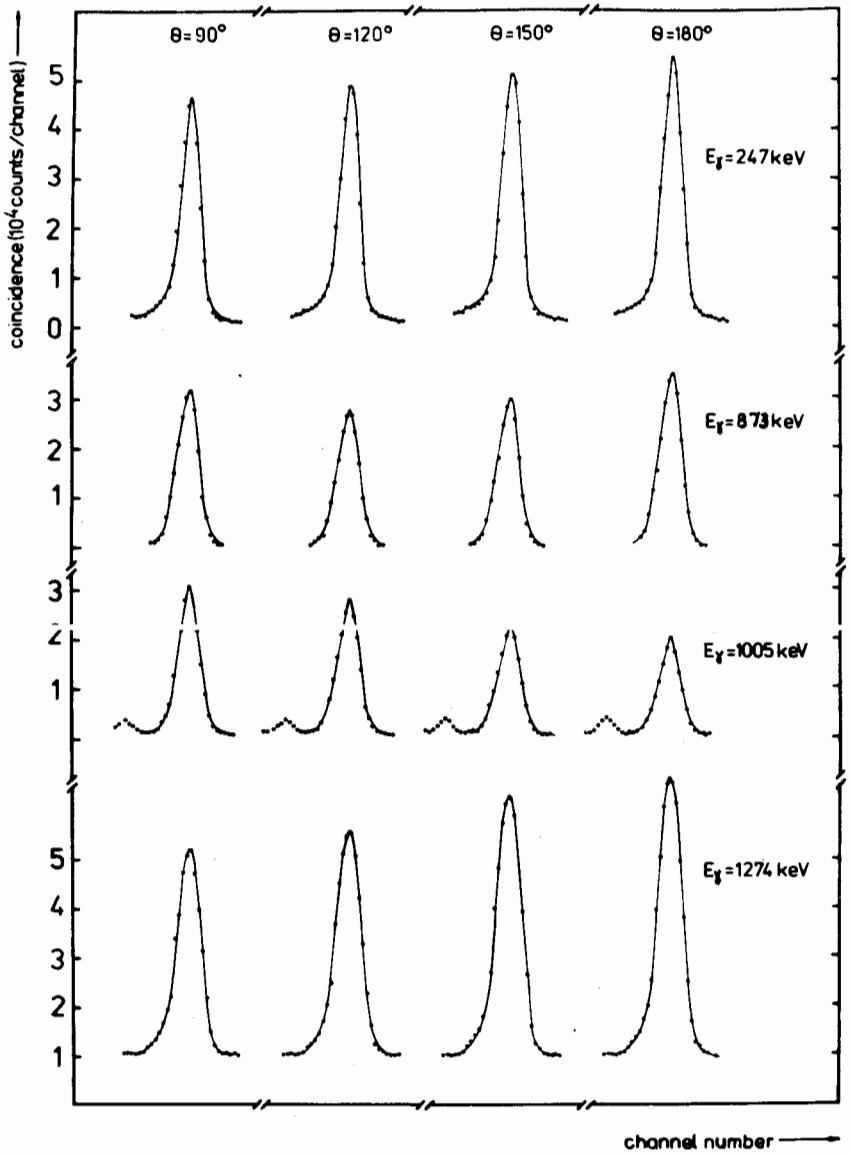
Electric field gradients on Gd nuclei in the Gd host

$V_{zz}^{exp} \times 10^{21}$ V/m^2	Measurement method	References
0.7±0.4	ME	/18/
0.87±0.08	ME	/19/
0.5±0.2	ME	/20/
1.05	ME	/21/
3.41±0.17*	CE	/22/
3.43±0.14	CE	/23/
3.25±0.24	IPAC	present paper

* The value is recalculated in ref.[23].

The figure illustrates, as an example, the coincidence spectra obtained from IPAC measurements for four (γ-γ) -cascades and for the following angles θ between the detectors: θ = 90°, 120°, 150°, and 180°. Using the data analysing program QUDIM[15], ω_0 was obtained from the least square fit of the functional

$$N(\theta_{i\ell}) = N_0\Big[1 + A_{22}\sum_{N=0}^{2} f_{22}^{NN}(\theta_{i\ell}) \sum_{n\geq 0}^{n_{max}} \frac{S_{nN}^{22}}{1+(n\omega_0\tau)^2} + A_{24}\sum_{N=0}^{2} f_{42}^{NN}(\theta_{i\ell}) \sum_{n\geq 0}^{n_{max}} \frac{S_{nN}^{24}}{1+(n\omega_0\tau)^2} + A_{42}\sum_{N=0}^{2} f_{42}^{NN}(\theta_{i\ell}) \sum_{n\geq 0}^{n_{max}} \frac{S_{nN}^{42}}{1+(n\omega_0\tau)^2} + A_{44}\sum_{N=0}^{4} f_{44}^{NN}(\theta_{i\ell}) \sum_{n\geq 0}^{n_{max}} \frac{S_{nN}^{44}}{1+(n\omega_0\tau)^2}\Big], \qquad (4)$$



Coincidences spectra γ-ray with the energy 123 keV with γ-rays of the energy 247, 873, 1005, and 1274 keV for angles between detectors being θ = 90, 120, 150, and 180°.

to the experimental data. Here $N(\theta_{i\ell})$ is the number of coincidences detected at a certain position of the crystal with respect to the detectors, the coefficients $f^{NN}_{k_1 k_2}(\theta_{i\ell})$ contain information on the relative positions of the detectors and the c-axis of the single crystal /16/. Taking into account the data of I, Q and τ for the 123 keV intermediate state of ^{154}Gd /24,25/ from the value of ω_g averaged over all cascades one obtains by eq. (3) the EFG value $V_{zz}^{exp} = (3.25 \pm 0.24) \cdot 10^{21} Vm^{-2}$, which is close to the value obtained by the Coulomb excitation method (Table 1). The lattice contribution to the EFG was calculated using the plane-wise summation method of de Wette /26/, which yields $V_{latt} = 0.177 \cdot 10^{20} Vm^{-2}$. Therefore $V_{latt}(1 - \gamma_\infty) = 1.35 \cdot 10^{21} Vm^{-2}$ and the ratio $V_{zz}^{exp} / V_{latt}(1 - \gamma_\infty) = 2.4$ corresponds to empirical rule (2), considering, that the PAC experiment does not determine the sign of V_{zz}.

3.2. EFG in Trifluorides of Rare-Earths

The rare earth trifluorides LaF_3, CeF_3, PrF_3, and NdF_3 crystallize into a hexagonal structure of the PCu_3 type with the D^4_{3d} space group /27/. The rare earth ions occupy positions with a monoclinic point symmetry (C_2).

The trifluorides SmF_3, EuF_3, and GdF_3 crystallize into an orthorhombic structure of the YAl_3 type with the D^{16}_{2h} space group /28/, and the rare earth ions occupy sites with the monoclinic point symmetry also. For both cases the point symmetry at rare earth sites is non-axial, therefore the parameter η should be non-zero.

In Table 2 the values of V_{zz} and η for the rare earth trifluorides obtained by the IPAC measurements are given. In addition, there are included the corresponding values of the earlier Mössbauer measurements. The values V_{zz} for isostructural compounds raise monotonously with the number of 4f electrons of the rare earth ions.

The uncertainties quoted at the experimental EFG values are mainly due to the inaccurate data of the quadrupole moment and of the half-life time of the 123 keV intermediate state in the ^{154}Gd nucleus.

The point charge model (PCM) has been assumed to be a good approximation to calculate the EFG in the trifluorides because of the small dipole polarizability of the fluorine ion F^- /3/. In this model the components of the lattice EFG tensor at a Gd^{3+} site may be expressed as the lattice sum

$$V_{ij} = \sum_{k\ell} Z(k) \left(3x_i(k,\ell)\, x_j(k,\ell) - \delta_{ij}\, r^2(k,\ell)\right) r^{-5}(k,\ell), \qquad (5)$$

Table 2

Electric field gradients V_{zz} in units $10^{21}\,Vm^{-2}$ and asymmetry parameters η on Gd nuclei in rare earth trifluorides

Compound	Experimental from IPAC meas. V_{zz}	η	Point charge model ** V_{zz}	η	Derived from EPR [7] V_{zz}	η	Lattice parameters [28] in Å a	b	c
LaF_3	4.2±0.2	0.3±0.2	1.60(1.57)	0.095(0.73)	2.74	0.12	7.186		7.352
CeF_3	4.6±0.2	0.3±0.2	1.64(1.61)	0.10 (0.73)	2.91	0.11	7.112		7.279
PrF_3	5.3±0.3	0.3±0.2	1.68(1.64)	0.10 (0.73)	3.06	0.105	7.075		7.238
NdF_3	5.2±0.3	0.3±0.2	1.69(1.65)	0.11 (0.73)	3.14	0.19	7.030		7.200
SmF_3	8.4±0.4	0.4±0.3	10.92	0.40			6.669	7.059	4.405
EuF_3	9.3±0.4	0.4±0.3	11.09	0.40			6.622	7.019	4.396
GdF_3	9.5±0.4	0.4±0.3	11.26	0.40			6.570	6.984	4.393
GdF_3	11.9±5.0	0.41±0.35	[18]	from Mössbauer measurements					
GdF_3	10.4±1.7	0.45±0.10	[40]						
GdF_3	12.4±0.3	0.7±0.10	[41]						
GdF_3	9.97±0.07	0.3978*)	[3, 19]						

*The principal axis is in a-c plane and directed under an angle 4° to the c-axis.
**For the light rare earth trifluorides are taken the data of Cheetham et al.(Zalkin et al.) [27].

where $Z(k)$ is charge and $x_i(k,\ell)$ is the i'th Cartesian coordinate of the k'th ion in the ℓ'th unit cell, $r(k,\ell)$ is the distance of this ion from the origin at the Gd^{3+} site of interest. The ionic positions in the unit cell were taken for the hexagonal compounds from [27,29], and for the orthorhombic ones from [3,29]. According to eq. (5) the direct summation was performed up to an ion distance of about 100 Å with respect to the ion of interest. The results of this calculations are given in Table 2.

The EFG values $V_{latt}(1-\gamma_\infty)$ from the PCM deviate significantly from the experimental V_{zz} values for the trifluorides of the light rare earth ions, whereas the asymmetry parameters calculated within the PCM depend sensitively upon the accuracy of the ion positions in the unit cell. We conclude that the PCM which proposes a completely ionic character of the lattice is insufficient for a full understanding of the EFG in these compounds. In [3] it was argued that including into consideration the overlap of the outer-shell electrons of the rare earth ions with those of the ligands and/or their polarizabilities will give no essentially better agreement with the experiment.

Recently [30], however, on the basis of the PCM and an induced-dipole model it has been calculated the spin-Hamiltonian parameters for Gd^{3+} - doped single crystals of rare earth fluorides. Considering effects of the admixture of excited 4f-states of Gd^{3+}, discussed widely by Wybourne [31] and Buckmaster [32], and taking into account appropriate polarizabilities of the F^- ions in a solid they were able to achieve a surprising good agreement of the calculated and the experimental spin-Hamiltonian parameters. These results, however, do not mean that effects such as overlap and covalency in this compounds do not play any role. Rather it is likely, that such effects are indirectly inclosed into the polarizability tensor used in their estimations and depending on the host lattice.

The discussion in paper [30] bases on the EPR measurements on Gd^{3+} in trifluorides of La, Ce, Pr and Nd [7], which confirm the more earlier results of Sharma [6] and Jones et al. [5]. It is of interest to connect the parameters b_2^m (m = 0,2) occurring in the spin Hamiltonian, which were measured by EPR on Gd^{3+}, with the parameters of EFG which are obtained by IPAC measurements. To get a quantitative relation between the b_2^m and the CEF parameters A_2^m it is necessary to estimate various non-S-contributions to the 4f electron ground state in Gd^{3+}. Although it has been stated [31], that the ion contribution solely cannot explain the full splitting of the ground state in Gd^{3+}, usually it was taken into account only Hutchinson's mechanism of third order in the spin-orbit interaction [33] and the relativistic contribution given by Wybourne [34].

$$b_2^\circ = \left(-\frac{12}{5}\,\frac{\zeta^3}{W_P^2 W_D}\langle r^2\rangle + \frac{56}{245}\,\frac{\zeta(R_{--}^2 - R_{++}^2)}{W_P}\right)(1-\sigma_2)A_2^\circ , \qquad (6)$$

here ζ is the one-electron spin-orbit coupling parameter, W_P and W_D are the energy separations between the ground state $^8S_{7/2}$ and the excited states $^6P_{7/2}$ and $^6D_{7/2}$, respectively, σ_2 considers the screening due to the $5s^2p^6$ electrons, $\langle r^2\rangle$ is the average of the operator r^2 for the 4f electron on Gd^{3+}, and R_{++}^2 and R_{--}^2 are relativistic integrals. Using the values quoted for instance in /35/ one obtains the quantitative relation $b_2^\circ(cm^{-1}) = 3.19\cdot10^{-5}\ A_2^\circ(cm^{-1}\,\text{Å}^{-2})$. Furthermore we assume the linear relation $b_2^\circ/A_2^\circ = b_2^2/A_2^2$, then the components of the EFG are given by

$$V_{zz} = 4A_2^\circ(1-\gamma_\infty)/e \quad \text{and} \quad \eta = A_2^2/A_2^\circ . \qquad (7)$$

The EFG values for the light rare earth fluorides derived from the EPR results /6,7/ are listed in Table 2 also. These values are about 30% smaller than those obtained by IPAC measurements. Taking into consideration the rough approximations we can conclude that by both methods are measured the same properties of the CEF which may be explained by a combined point charge and induced dipole model rather than by the PCM solely.

One of the most direct methods to measure the EFG is the nuclear quadrupole resonance (NQR). Andersson and Procter /8/ have performed NQR measurements on ^{139}La in LaF_3 at room temperature, and they obtained the quadrupole interaction constant to be $eV_{zz}Q/h = 16.11$ Mc/s which yields with the quadrupole moment of ^{139}La in its ground state $Q = 0.22(3)$ b /36/, the EFG at the lanthanum nucleus $V_{zz} = 3.03\cdot10^{21}Vm^{-2}$. The asymmetry parameter was find out to be $\eta = 0.804$. Considering the difference in the ion radii of La^{3+} and Gd^{3+}, the EFG value derived from NQR confirms the results of our IPAC measurements.

Recently Reddy and Erickson /9/ have studied the ground state of Pr^{3+} in LaF_3 by NQR. Because the ground state is a singlet there is no first order hyperfine interaction, and the Hamiltonian can be given by

$$\mathcal{H} = D(I_z^2 - 1/3\ I(I+1)) + E(I_x^2 - I_y^2) - \vec{H}\gamma_t\vec{I}, \qquad (8)$$

where $\vec{H}$ is the magnetic field, γ_t is the diagonal gyromagnetic tensor, the parameters D and E consist of three terms: firstly, the second-order hyperfine interaction, which dominates and can be calculated from CEF wave functions (if available) or estimated from the anisotropic paramagnetic shift of the resonance lines in the presence of a magnetic field, secondly, the contribution of the 4f electrons in Pr^{3+}, which may be neglected because of it gives only a value of about 10^{-6} cm^{-1}

using the wave functions from /37/, and thirdly the lattice contribution. Applying the measured quantities D = 4.185 Mc/s and E = 0.146 Mc/s /9/, which are in accordance with values given earlier by Teplov /38/, and those of the second-order hyperfine contribution D_a = 3.132 Mc/s and E_a = 0.596 Mc/s /9/, and using the screening parameter σ_2 = 0.745 /39/ and the quadrupole moment Q = 0.024 b or 0.0589 b /36/ for ^{141}Pr one obtains the EFG, at the site of the Pr nucleus which substitutes La in LaF_3, by the relation

$$V_{zz} = D_{latt}\,4I(2I-1)(1-\sigma_2)/3eQ, \quad D_{latt} = D - D_a \qquad (9)$$

to be $V_{zz} = 6.17\cdot10^{21}$ or $2.51\cdot10^{21}\,Vm^{-2}$, respectively, and η = = 0.43. It is very interesting to compare the components of the EFG tensor obtained by the IPAC measurements with those, which can be derived from the results of a systematic analysis of the optical absorption spectra from trivalent rare earth ions in the LaF_3 host lattice /10/. On the basis of the CEF Hamiltonian for the C_2 point symmetry at the site of the rare earth ions a fit procedure of the optical spectra yields all the fourteen CEF parameters for nine different rare earth ions in LaF_3. With the assumption that the substitution of a lanthanum ion in LaF_3 by a rare earth ion does not change considerably the CEF at this lattice site, from the CEF parameters $B_\ell^m = \rho_\ell A_\ell^m$ can be separated the rare earth ion dependent, but host independent modified radial integrals ρ_ℓ, which are tabulated in /10/, from the parameters A_ℓ^m characterizing the CEF behaviour in the host lattice of LaF_3. The quantities A_ℓ^m are assumed to be independent on the peculiarities of the rare earth ions and are averaged over the rare earth series. Using the resulting values $A_2^\circ = -1115\ \text{Å}^{-2}\ cm^{-1}$ and $A_2^2 = -458\ \text{Å}^{-2}\ cm^{-1}$ the components of the EFG at the lanthanum site in LaF_3 are given by eq. (7) to be $V_{zz} = 4.20\cdot10^{21}Vm^{-2}$ and $\eta = 0.41$, respectively. This values are very close to those obtained by the IPAC method. Furthermore, by analysing the optical absorption spectrum and the paramagnetic susceptibility data of NdF_3 the CEF parameters for the site of the Nd^{3+} ion have been found /11/. Taking into account their values $B_2^0 = -203\ cm^{-1}$ and $B_2^2 = -90\ cm^{-1}$ and considering the modified radial integral ρ_2 given in /10/ the components of the EFG tensor at the Nd^{3+} site in NdF_3 can be derived to be $V_{zz} = 4.48\cdot10^{21}cm^{-2}$ and $\eta = 0.44$, which again correspond very close with the results from the IPAC measurements.

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Градиенты электрического поля на ядрах ^{111}Cd в монокристаллах гадолиния и трифторидов редкоземельных элементов

Методом интегральных возмущенных угловых корреляций измерены градиенты электрических полей на ядрах ^{111}Cd в монокристаллах гадолиния и трифторидов редкоземельных элементов: LaF_3, CeF_3, PrF_3, NdF_3, SmF_3, EuF_3, GdF_3. Экспериментальные величины сравниваются с расчетами, проведенными по модели точечных зарядов, и результатами других измерений, таких, как мессбауэровская спектроскопия, электронный парамагнитный резонанс, ядерный квадрупольной резонанс и оптическое поглощение. Градиенты электрического поля для ^{111}Cd в трифторидах легких редкоземельных элементов недостаточно хорошо описываются моделью точечных зарядов.

Работа выполнена в Лаборатории ядерных проблем ОИЯИ.

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Budzynski M. et al. E14-83-605

Electric Field Gradients at ^{111}Cd in Gadolinium and Rare Earth Trifluoride Single Crystals

Electric field gradients at the ^{111}Cd nuclei in monocrystals of gadolinium and rare earth trifluorides: LaF_3, CeF_3, PrF_3, NdF_3, SmF_3, EuF_3, and GdF_3 have been measured by the method of integral perturbed angular correlation. The experimental data have been compared with those of point charge model calculations and with the results of other experiments such as Mössbauer spectroscopy, electron paramagnetic resonance, nuclear quadrupole resonance, and optical absorption. The results obtained for ^{111}Cd in trifluorides of the light rare earth elements allow one to conclude that the field gradients cannot be explained within the point charge model.

The investigation has been performed at the Laboratory of Nuclear Problems, JINR.

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