Calculation of electric field gradient at nuclei in crystals from x-ray diffraction data

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An attempt is made to calculate the electric field gradient at the Fe nucleus in hematite (α-Fe_2O_3) and sodium nitroprusside ($Na_2[Fe(CN)_5NO] \cdot 2H_2O$) from x-ray diffraction experimental data. The results are compared with the ratio of the quadrupole splitting in the gamma-resonance spectra of these two compounds. Also calculated are the quadrupole moment of the ^{57}Fe nucleus excited to the 14.4 keV level; the moment found is $Q = 0.14 \pm 0.02$ b.

INTRODUCTION

The presently employed x-ray diffraction method makes it possible to determine with a resolution ~ 0.1 Å, in the form of a Fourier series, the distribution of the electron density $\rho(\mathbf{r})$ of the ground state of a crystal.[1,2] The moduli of the Fourier transforms of $\rho(\mathbf{r})$ [of the structural amplitudes $F(\mathbf{s})$] are recalculated from the intensities of the reflections of coherently scattered radiation, subject to correction of a number of effects that influence the results, such as multiple, Compton, and thermal diffuse scattering, extinction, absorption, and anomalous scattering. The $F(\mathbf{s})$ phases are calculated by using any of a number of theoretical models. The availability of the "experimental" electron density stimulates development of solid-state theory methods in which $\rho(\mathbf{r})$ is used.[3,4]

One must be assured, however, that this electron density is not distorted by uncorrected experimental effects and by the model approximations used for the reduction of diffraction data. To be certain of sufficient accuracy, the data obtained can be compared with results of an independent experiment. In the present paper we have calculated, for such a comparison, the component eq_{zz} of the electric field gradient (EFG) at Fe nuclei in crystals of sodium nitroprusside (SNP) $Na_2Fe[(CN)_5NO] \cdot 2H_2O$ (space group *Pnnm*) and hematite α-Fe_2O_3 (space group $R\,\bar{3}c$). The initial data for the calculation were the results of high-precision x-ray diffraction experiments on these crystals.

In hematite α-Fe_2O_3 the symmetry of the position of the iron ion (D_{3d}) is such that the z axis of the hexagonal cell and the principal z axis of the EFG tensor coincide. The components of the EFG at the Fe nucleus are connected by the relation $eq_{xx} = eq_{yy} = -\frac{1}{2}eq_{zz}$, and the EFG is fully described by one component eq_{zz}. In the SNP crystal the iron ion occupies a particular position, whose point symmetry can be approximately described as C_{4v}. It can therefore be assumed that $eq_{xx} \approx eq_{yy}$ and that here, just as in hematite, the EFG is characterized by one component in the principal-axes system (the EFG asymmetry parameter in SNP is $(eq_{xx} - eq_{yy})/eq_{zz} \approx 0.01$, Ref. 5). The following relation is then valid:

$$\alpha \equiv (eq_{zz})_{\mathrm{SNP}}/(eq_{zz})_{\mathrm{Fe_2O_3}} = \Delta_{\mathrm{SNP}}/\Delta_{\mathrm{Fe_2O_3}}. \tag{1}$$

Here Δ_{SNP} and $\Delta_{\mathrm{Fe_2O_3}}$ are the values, measured by gamma-resonance spectroscopy (GRS), of the quadrupole splitting of the spectral lines.[6] For the ^{57}Fe nuclei in the indicated compounds, the value of α can be easily obtained from GRS data known in a wide range of temperatures, and Eq. (1) makes it possible to estimate directly the accuracy of the eq_{zz} values calculated from x-ray diffraction data. For crystals that differ so greatly in structure, one can hardly expect the obtained eq_{zz} to differ from the actual ones by one and the same factor, and satisfaction of condition (1) means that the values of eq_{zz} have been correctly determined. Moreover, calculation makes it possible to obtain from the distribution of the electron density not only the magnitude but also the sign of eq_{zz}; measurements by the GRS method in single crystals make it also possible to determine experimentally the sign of the constant Δ. The leads to another possibility of verifying the accuracy of the recovery of the electron density from x-ray-diffraction data. Recognizing that for the crystals in question we have $\Delta = \frac{1}{2}e^2 q_{zz} Q$, where Q is the ^{57}Fe quadrupole moment in a state excited to the 14.4 keV level, we can determine the magnitude and sign of Q from the obtained value of eq_{zz} and from the experimentally observed Δ. This is of interest for nuclear physics, since the value of Q for ^{57}Fe has not yet been determined reliably.

EXPERIMENTAL DATA AND CALCULATION PROCEDURE

In the general case, the EFG is a tensor of second rank, which has in the principal-axes system two independent components ($\Sigma_{ii} eq_{ii} = 0$), defined by the expression

$$eq_{ij} = -e \int_{-\infty}^{\infty} \left\{ (3r_i r_j - \delta_{ij}|\mathbf{r}|^2) \frac{1}{|\mathbf{r}|^5} \right\} \sigma(\mathbf{r})\, dV. \tag{2}$$

Here r_i is the projection of the vector $\mathbf{r}$ on the axis $i = x,y,z$, and

$$\sigma(\mathbf{r}) = \rho(\mathbf{r}) + \sum_i z\delta(\mathbf{r} - \mathbf{r}_i)$$

represents (the electronic and nuclear, respectively) charge density in the crystal. An x-ray diffraction experiment yields the time-averaged electron-density distribution function $\langle \rho(\mathbf{r}) \rangle$ which is generally dependent on temperature. Therefore the EFG calculated directly from the "experimental" function $\langle \rho(\mathbf{r}) \rangle$ will depend on the degree of "thermal smearing" of the quadrupole deformation of the electron distribution relative to the considered nucleus. This smearing is determined by the character and the magnitude of the

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thermal motion of the atoms and can distort these calculation results. To calculate the EFG by this method it is therefore desirable to use low-temperature diffraction data (or the pseudostatic electron density reconstructed from the parameters of a certain analytic expansion of $\langle\rho(\mathbf{r})\rangle$.[1] On the other hand, the relaxation times of the resonance experiments are as a rule longer by six or seven orders than the period of the atom vibrations in crystals ($t\sim 10^{-13}$–10^{-14} s). The thermal motion of the atoms should have practically no effect on the hyperfine interaction constant in GRS, at any rate so long as the oscillation amplitudes are much smaller than the characteristic interatomic distances in the crystals. Indeed, as shown by the results of gamma-resonance investigations,[7,8] the magnitude and sign of the EFG at the iron nucleus in α-Fe_2O_3 and SNP remain unchanged in a large temperature interval.

It is clear hence that the mean value of the EFG at the nucleus, which is involved in the GRS, will generally speaking not be equal to the EFG at the time-averaged position of the nucleus as calculated from $\langle\rho(\mathbf{r})\rangle$. The difference between them will decrease with temperature.

We have calculated the EFG from x-ray diffraction data obtained at 153 K with the automatic four-circle diffractometer "Sinteks-R2$_1$" (the measurements were made at the Institute of Organometallic Compounds of the USSR Academy of Sciences jointly with Yu. T. Struchkov and M. Yu. Antipin). The single crystals of both compounds were spherical ($r = 0.15$ mm). We used Mo $K\alpha$ radiation, a graphite monochromator, $\theta/2\theta$ scanning of the diffraction peaks, and ψ scanning of some of them to eliminate multiple reflections.[1] For α-Fe_2O_3 we measured 4354 reflection over the entire Ewald sphere to 1.36 Å^{-1}. Averaging of those equivalent in symmetry left 527 independent reflections corrected further for absorption, isotropic extinction, and anomalous scattering. The position and thermal (in the harmonic approximation with allowance for the anisotropy of the vibrations) structure parameters used to calculate the $F(\mathbf{s})$ phases were refined by least squares using large-angle reflections with $\sin\theta/\lambda > 1.0$ Å^{-1} (Ref. 1) to $R = 0.0181$, $R_w = 0.0246$, $S = 1.7044$. In x-ray structure analysis it is customary to estimate the result of optimization of the crystal model by means of the normalized average deviation

$$R=\sum_{\mathbf{s}}^{n} \big|\,|F(\mathbf{s})|-|F_{\text{calc}}(\mathbf{s})|\,\big| \Big/ \sum_{\mathbf{s}}^{n} |F(\mathbf{s})|,$$

the normalized standard deviation

$$R_w=\Big\{\sum_{\mathbf{s}}^{n} w(\mathbf{s})\,[\,|F(\mathbf{s})|-|F_{\text{calc}}(\mathbf{s})|\,]^2 \Big/ \sum_{\mathbf{s}}^{n} w(\mathbf{s})\,|F(\mathbf{s})|^2\Big\}^{1/2}$$

and the model-refinement quality index

$$S=\Big\{\sum_{\mathbf{s}}^{n} w(\mathbf{s})\,[\,|F(\mathbf{s})|-|F_{\text{calc}}(\mathbf{s})|\,]^2/(n-m)\Big\}^{1/2}.$$

Here $F_{\text{calc}}(\mathbf{s})$ is the structural amplitude that represents the model of the crystal, $w(\mathbf{s})$ is the statistical weight of the measurement, n is the number of reflections included in the refinement, and m is the number of parameters of the model. We also measured 12676 reflections from the SNP crystal up to $\sin\theta/\lambda < 1.15$ Å^{-1}, of which 7884 reflections in the interval 0–0.64 Å^{-1} were measured over the entire Ewald sphere, and the remaining 4832 reflections were measured in two octants of reciprocal space ($h\bar{k}l$ and $\bar{h}\bar{k}\bar{l}$). After averaging the symmetrically equivalent ones, 3777 reflections were left, corrected for absorption, isotropic extinction, and anomalous scattering. The positional and thermal parameters of these non-hydrogen atoms were refined to fit reflections with $\sin\theta/\lambda > 0.65$ Å^{-1}, the positions of the weakly scattering H atoms were obtained from a difference synthesis, and the coordinates of these atoms were next recalculated, retaining the O–H directions,to the average neutron-diffraction lengths of the bonds in the water molecule, equal to 0.967 Å (Ref. 9). The refinement indices are equal to $R = 0.0137$, $R_w = 0.0147$, $S = 1.43$. A more detailed description of the experiment and of the data reduction was published separately.[10,11]

The EFG calculation was based on an approach proposed in Ref. 12. We express the total charge density $\sigma(\mathbf{r})$ in (2) in the form

$$\sigma(\mathbf{r})=\sigma_0(\mathbf{r})+\delta\rho(\mathbf{r}), \tag{3}$$

where $\sigma_0(\mathbf{r})$ is the total charge density in a hypothetical crystal made up of an aggregate of spherical atoms located at the lattice sites ("procrystal"), $\delta\rho(\mathbf{r})$ is the deformational electron density, including all the changes that took place in the electron density of the procrystal when the real crystal was formed (i.e., when the chemical bond was formed). It follows then from (2) and (3) that

$$eq_{ij}=eq_{ij}^{0}+e\delta q_{ij}, \tag{4}$$

where eq_{ij} is the EFG due to the distribution of the electrons and nuclei in the procrystal: this contribution is easily calculated using tabulated data[13] if the crystal structure is known[12]; $e\delta q_{ij}$ is the EFG due to the deformation of the electron density. The value of $e\delta q_{ij}$ can be calculated by using the Fourier transform of an expression similar to (2) but written for the deformation EFG:

$$e\delta q_{ij}=\frac{4\pi e}{3V}\sum_{\mathbf{s}}\Big\{\frac{3s_is_j-\delta_{ij}|\mathbf{s}|^2}{|\mathbf{s}|^2}\Big\}\,\delta F(\mathbf{s})\exp\{-2\pi i\mathbf{s}\mathbf{r}\}, \tag{5}$$

where $\delta F(\mathbf{s}) = F(\mathbf{s}) - F_{calc}(\mathbf{s})$ is the difference between the x-ray structure amplitudes (experimental and calculated) for the procrystal. It is shown in Refs. 14 and 15 that the $e\delta q_{ij}$ calculated from expression (5) in first approximation can be regarded as a representative of the static electron density. Therefore, by calculating from the time-averaged positions of the nuclei the contribution of the eq_{ij}^{0}, we can reconcile the resultant EFG (4) with the spectroscopic data.

The quantity $\delta F(\mathbf{s})$ in (5) is subject to statistical errors that influence the accuracy of the calculated $e\delta q_{ij}$. To decrease the influence of the random errors, we used in the summation of the series (5) a filtering procedure based on the Tikhonov regularization procedure (Ref. 16) and consisting of introducing into the sum (5) filtering factors of the form[17]

$$M_{\mathbf{s}}=\begin{cases} |\delta F|^2/[\,|\delta F|^2+\sigma^2(\delta F)\,], & |\delta F|\geqslant(\beta+1)\sigma(\delta F),\\ \dfrac{|\delta F|^2}{|\delta F|^2+\sigma^2(\delta F)}\Big[\dfrac{|\delta F|}{\sigma(\delta F)}-\beta\Big], & \beta\sigma(\delta F)<|\delta F|<(\beta+1)\sigma(\delta F),\\ 0, & |\delta F|\leqslant\beta\sigma(\delta F). \end{cases} \tag{6}$$

(β is a filtering parameter that depends on the error-distribution law). The expression for the components $e\delta q_{ij}$ with allowance for the filtering takes the form

$$e\delta q_{ij}=\frac{4\pi e}{V}\sum_{s}\left\{\frac{h_ih_j}{|\mathbf{s}|^2}-\frac{(\mathbf{a}_i\mathbf{a}_j)}{3}\right\}M_s[\delta F(\mathbf{s})]\exp\{-2\pi i\mathbf{sr}\},\tag{7}$$

where $\mathbf{a}_i$ are the vectors of the direct lattice, and $h_i = h,k,l$. The corresponding expression for the variance $\sigma^2(e\delta q_{ij})$ takes for the considered centrosymmetric crystals the form

$$\sigma^2(e\delta q_{ij})=\left(\frac{4\pi e}{V}\right)^2\times 4\sum_{s}M_s\left\{\frac{h_ih_j}{|\mathbf{s}|^2}-\frac{(\mathbf{a}_i\mathbf{a}_j)}{3}\right\}^2\sigma^2[\delta F(\mathbf{s})]\cos^2(2\pi\mathbf{sr}).\tag{8}$$

Expressions (7) and (8) determine $e\delta q_{ij}$ and $\sigma^2(e\delta q_{ij})$ in the reciprocal-lattice coordinate frame and can be easily transformed to the principal axes connected with the investigated nucleus. It should be noted that if the EFG is calculated using reciprocal space, automatic account is taken of the symmetry and of the long-range order in the crystal, inasmuch as in **r**-space, to ensure convergence of the integral in (2), it would be necessary to use in the calculations a large number of coordination spheres that surround the given nucleus.

RESULTS

The EFG component $e\delta q_{zz}$ at the Fe atom with coordinates (0;0;0.35520) in an α-Fe_2O_3 crystal was calculated from Eq. (7), and its variance was determined in accordance with (8). To exclude the influence of the filtering procedure on the result, the calculations were performed for various values of the parameter β. It was found that when β is varied in the interval $1\leqslant\beta\leqslant 2$ the value of $e\delta q_{zz}$ remains unchanged within one mean-squared deviation. At the same time, filtering decreases the error by an approximate factor of 2. The most reliable result, obtained at $\beta = 1.7$, when the condition

$$e\delta q_{xx}=e\delta q_{yy}=-{}^1/_2 e\delta q_{zz}$$

is satisfied almost exactly, is $e\delta q_{zz} = (0.33 \pm 0.05)\cdot 10^{22}$ V/m. The contribution eq^0_{zz} made to the EFG by spherical atoms turned out to be an order of magnitude smaller than the mean squared deviation of $e\delta q_{zz}$.

In the SNP crystal, the largest EFG component eq_{zz} corresponds to the Fe–NO direction in the *ab* plane, and one of the remaining equal components corresponds to the direction along the crystallographic *c* axis. This simplifies the calculations greatly. Calculation of eq_{zz} using Eq. (7) yielded for the EFG at the Fe nucleus a value $e\delta q_{zz} = (1.17 \pm 0.14)\cdot 10^{22}$ V/m. The term eq^0_{zz} in (4), which is due to the contribution made to the EFG by the atoms surrounding the investigated nucleus, is negligibly small. The value of α [Eq. (1)] obtained on the basis of low-temperature experimental structural amplitudes for α-Fe_2O_3 SNP turned out to be 3.55 ± 0.11. A special measurement of the quadrupole splitting of a very pure α-Fe_2O_3 sample yielded $\Delta = 0.48 \pm 0.02$ mm/s (at 295 K). In conjunction with the SNP data obtained in Ref. 8 ($\Delta_{SNP} = 1.7170 \pm 0.0040$ mm/s at 100 K) this leads to $\alpha_{GRS} = 3.58 \pm 0.14$.

On the basis of the $e\delta q_{zz}$ calculated from x-ray diffraction data and of the experimentally measured values of the quadrupole splitting in α-Fe_2O_3 and SNP one can determine the quadrupole moment of the ^{57}Fe nucleus excited to the 14.4 keV level. This moment is equal to $Q = (0.14 \pm 0.02)\cdot 10^{-28}\, m^2$.

DISCUSSION OF RESULTS

Calculations of EFG at nuclei in crystals were based for a long time on the static ion model of the crystal.[6,18] The nonzero contribution to the EFG obtained when the surrounding of the nucleus is not cubic was obtained, and added to it was the EFG produced by the electrons of the partially filled shells of the investigated atoms, and also a component due to the dipole and higher deformations of the electron shells of the neighboring anions.[19,20] Since the ion model does not give the complete picture of the electron distribution and leads to a wrong electrostatic interaction of the nucleus with the surroundings, correction coefficients were included in the model, viz., Sternheimer factors calculated with by multiparticle perturbation theory or by a variational or other methods.[18] Unfortunately, this method of calculating the EFG leads to contradictory results and necessitates a more complete and consistent allowance for the peculiarities of the electronic structure of crystals. In particular, it was emphasized[21] that the EFG calculation must include, in a self-consistent manner, the effects of long-range action, the non-sphericity of the atomic electron clouds, their overlap, and the electron transfer. This would obviate the use of the Sternheimer screening corrections by proceeding to calculate the EFG from first principles. At the present stage of development of methods for calculating the electron density of crystals, however, this problem cannot be solved in such a formulation. For the time being we can calculate EFG only for clusters made up of a small number of atoms,[22] and the influence of the electrostatic field of the crystal atoms surrounding the cluster is imitated by point charges and multipole moments of the ions. Such an approach would probably be justified in ionic crystals. But in framework compounds with partially covalent multicenter chemical bonds the fragments that lend themselves to calculation do not make it possible to take into account the overlap of the electron clouds of the atoms in these compounds and of the rest of the crystal. For example, it follows from a cluster calculation for the α-Fe_2O_3 crystal[22] that the d_{z^2} orbital of Fe is not occupied by electrons, thus contradicting the data of Goouden-ough[23] and disagreeing with the results of Ref. 24. In that paper the approximation of overlapping electron clouds of the ions was used for a consistent calculation of local, nonlocal (with orthogonalization of the orbitals), and long-range crystalline effects that determine the EFG at the nucleus of the cation in α-Fe_2O_3, but the redistribution of the electron density when the crystal is made up of the Fe^{3+} and O^{2-} ions was not taken into account. The obtained value $0.81\cdot 10^{21}$ V/m^2 at the Fe nucleus yielded for $Q = 0.082\cdot 10^{-28}$ m^2 (data of a nonempirical calculation of the $FeCl_2$ and $FeBr_2$ molecules[21]) a quadrupole-interaction constant approximately one-sixth the experimental value. The discrepancy between the theoretical and spectroscopic data can be eliminated only by assuming that the d_{z^2} orbitals of the Fe atoms that form the state a_1 have an electron population 13.6% larger

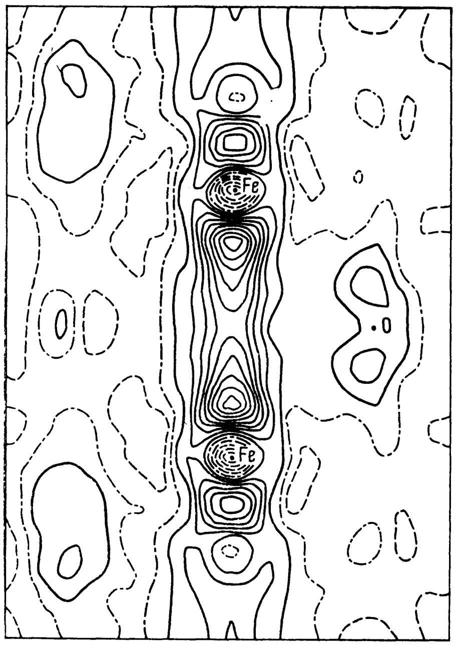

FIG. 1. Section of deformation electron density $\delta\rho(\mathbf{r})$ in α-Fe_2O_3 by the plane passing through the z axis and the O atom. The isolines are drawn in steps of 0.2 el·Å^{-3}. The positive deformation density is marked by solid lines, the negative by dashed lines, and the zero level by dash-dot lines.

than the remaining d orbitals. The validity of this assumption is confirmed by the experimental distribution of the deformation density $\delta\rho(\mathbf{r})$ near the cations in α-Fe_2O_3 (Ref. 11), which demonstrates unambiguously the predominant occupation of the state a_1 by electrons (Fig. 1), whereas the calculation of Ref. 22 does not lead to a covalent interaction between the cations along the z axis of the cell.

The situation with the calculations of EFG in crystals led a substantial scatter of the data on the quadrupole moment of the ^{57}Fe nucleus excited to the 14.4 keV level. This moment has not been experimentally determined to this day, in view of the short lifetime of the excited level. A theoretical calculation of Q from the structure of the ^{57}Fe nucleus yields $Q = (0.16 \pm 0.02)\cdot 10^{-28}$ m^2 (Ref. 25). Usually, however, Q is estimated from the measured quadrupole-interaction constant, after first calculating the EFG. Such estimates were made many times for α-Fe_2O_3. At first most workers considered the value $Q = (0.28 \pm 0.01)\cdot 10^{-28}$ m^2 to be reliably established by this method,[19] but later values $Q = (0.15 \pm 0.20)\cdot 10^{-28}$ m^2 were obtained.[26] It was noted in Ref. 2 that lower values of the quadrupole moment of ^{57}Fe followed from calculations for compounds of divalent iron, and higher ones for trivalent compounds. This pointed clearly to defects of the parametric ion model on which the EFG calculations were based, and stimulated the aforementioned more consistent and more complicated calculations,[21,22] according to which Q is in the range $(0.082$–$0.108)\cdot 10^{-28}$ m^2.

Thus, the earlier investigation did not make it possible to establish finally the value of the quadrupole moment of ^{57}Fe, in view of the limitation of the contemporary status of the methods for calculating the electronic structure of solids. Yet the solution of this problem remains important for nuclear physics and Mossbauer spectroscopy. Therefore the possibility of calculating the EFG from data on x-ray diffraction, and by the same token circumventing the difficulties of the non-empirical calculation, is quite enticing. That this approach is feasible in principle was noted by Stewart,[27] who showed subsequently[14] that the resolution of the details of the electron density obtained in experiment is sufficient to calculate EFG accurate to 10–15%. In several studies attempts were made to determine the EFG by diffraction.[28–30] These papers stressed procedure, so that it is difficult to asses the reliability of their results, owing to the variety of the methods used to reduce the experimental data. The authors of Refs. 28–30 reached the conclusion that the sign of the EFG is almost always correctly determined, and that the accuracy of the EFG depends on the accuracy of the initial diffraction data.

The diffraction data used in our calculation made it possible to determine the deformation electron density $\delta\rho(\mathbf{r})$ with an error 0.05 el·Å^{-3} in the chemical-bond region and 0.10 el·Å^{-3} at the Fe nucleus. It is important that the EFG at the nucleus depends not on the total electron density surrounding the nucleus, but only on its quadrupole deformation relative to this nucleus. The region of this deformation is located at a distance 0.12–0.2 Å from the nucleus, and the error of $\langle\delta(\mathbf{r})\rangle$, which increases as the nucleus is approached (Ref. 1) still does not obscure the singularities of $\delta\rho(\mathbf{r})$. As seen from the foregoing results, the actual accuracy with which the EFG of α-Fe_2O_3 and SNP crystals was determined by diffraction was 12–15% at 153 K.

The SNP crystals have a standard quadrupole splitting of the gamma-resonance spectra: when the temperature varies between 100 and 295 K, the value of Δ_{SNP} changes only by 0.8% (Ref. 8). The value of $\Delta_{Fe_2O_3}$ for one and the same pure hematite crystal sample is also independent of temperature,[7] but the literature cites for different samples differing experimental values. At room temperature, thus, according to data of various workers, the value of $\Delta_{Fe_2O_3}$ is: 0.48 ± 0.03 mm/s (Ref. 31), 0.44 ± 0.02 mm/s (Ref. 19), and 0.42 ± 0.02 mm/s (Ref. 7); for 130 K, Ref. 7 cites 0.42 ± 0.02 mm/s. The observed changes of Δ are apparently due to small differences in the sample composition, caused by the synthesis conditions. The average of our data and the published ones, $\Delta_{Fe_2O_3} = 0.45$ mm/s and $eq_{zz} = 0.33\cdot 10^{22}$ V/m^2, leads to $Q = 0.13\cdot 10^{-28}$ m^2, which agrees within a mean squared deviation with the quadrupole moment obtained above for the ^{57}Fe nucleus.

CONCLUSION

The electric field gradients at the Fe nuclei in α-Fe_2O_3 and sodium nitroprusside crystals, calculated from x-ray diffraction data, agree well with the experimental results obtained for these compounds by the GRS method. It can therefore be stated that the distribution of the electron density in these crystals is well described with the aid of an analysis of the x-ray structure amplitudes and can be used in calculations of the macroscopic properties of these crystals. The agreement between quantities obtained by totally independent experimental methods (GRS and x-ray diffraction analysis) suggests a value $Q = (0.14 \pm 0.02)\cdot 10^{-28}$ m^2 for a ^{57}Fe nucleus excited to an energy level 14.4 keV.

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