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Computation of Magnetic Field Dependence of the Dipolar Interaction Frequency of Oxygen Ion Center in CaF_2 Crystal

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ABSTRACT

This work is concerned with the analyzing and studying the magnetic field dependence of the dipole-dipole interaction frequency for an Oxygen ion center and it's neighbours. Six groups of ions are described by their geometrical part tensors and analyzed for two different combinations of axes in the presence of an external magnetic field. Discussion is given for the interpretation of these results.

دراسة الاعتماد على شدة المجال المغناطيسي لتردد ثنائي القطب المغناطيسي لأيون الأوكسجين في بلورة فلوريد الكالسيوم

الملخص

اعتمد العمل تحليل ودراسة اعتماد تردد ثنائي القطب المغناطيسي لأيون الأوكسجين المندمج في بلورة فلوريد الكالسيوم على شدة المجال المغناطيسي آخذين بنظر الاعتبار الأفعال المتبادلة ما بين الأيون المركزي وست مجموعات من أيونات الفلورين المجاورة مع حساب عناصر الممتدة لكل مجموعة ولمنظومتين من الإحداثيات، ومن ثم دراسة التغير في التردد بوجود مجال مغناطيسي خارجي، مع مناقشة وتعليل النتائج.

INTRODUCTION

The magnetic dipolar interaction is usually the most important cause of line broadening in a rigid lattice of magnetic dipoles. The magnetic field $\Delta\vec{B}$ seen by a magnetic dipole moment $\vec{m}_i$ due to a magnetic dipole $\vec{m}_j$ at a point $\vec{r}_{ij}$ from the first dipole is (Kittle, 1976):

$$\Delta\vec{B} = \frac{3\mu_o\,[(\vec{m}_j \cdot \vec{r}_{ij})\vec{r}_{ij} - \vec{m}_j\, r_{ij}^2]}{4\pi r_{ij}^5} \qquad (1)$$

Where:

$\mu_o = 4\pi \times 10^{-7}$ volt . sec/ Amper . meter (permeability of free space).

The local field at a given site will depend on the arrangement of the neighbours and the directions of their dipole moments. In the presence of external magnetic field $\bar{B}$, the local field at each ion must be added in a vector form to it, giving a displacement to the resonance interaction frequency of each ion. This result gives us a measure of the width of the spin resonance line.

The energy of interaction between two point magnetic dipoles having moments $\bar{m}_i = -g_i \beta \bar{S}_i$ and $\bar{m}_j = -g_j \beta \bar{S}_j$ located a distance r_{ij} away from each other can be written in operator form as (Abragam and Bleaney, 1970),

$$E_{dd} = g_i g_j \beta^2 r_{ij}^{-3}[\bar{S}_i \cdot \bar{S}_j - 3r_{ij}^{-2}(\bar{S}_i \cdot \bar{r}_{ij})(\bar{S}_j \cdot \bar{r}_{ij})] \qquad (2)$$

Where β is the Bohr magneton. The second term in equation (2) is strongly dependent on the orientation of $\bar{B}$ relative to the principal axes of the crystal (Poole and Farah, 1971).

Recently, a number of papers have dealt with computations of angular dependence of dipolar interaction frequency DIF between magnetic dipole moments of Oxygen ion center in CaF_2 crystal (Kasir, 1993) and computations of angular and magnetic field dependence of DIF of interstitial hydrogen atoms in CaF_2 crystal (Kasir, 1994).

This paper is concerned with computations of the magnetic field dependence of the dipolar interaction between Oxygen ion center and six group of fluorine ions in CaF_2 crystal.

PROCEDURE AND RESULTS

In this work, the model postulated for the oxygen center is shown in Fig.1 and it consists of pair of oxygen ions O^{-2} replace two adjacent fluorine F^- ions with a positive hole trapped on each oxygen ion to form an oxygen center which consists of two adjacent O^- ions. These types of oxygen centers may occur either naturally or produced by irradiation (Callow, 1977).

Taking into account the nearest and next-nearest neighbours, one may distinguish six different classes of ions, each class represents a state of group of equivalent ions. Calculations have been done to determine the position vector $\bar{r}$ and the direction cosines of $\bar{r}$ for each class of ions, taking into account that the distance between fluorine ions in CaF_2 crystals is 0.2725 nm, and then combined with the normalized frequency, to get the geometrical parts of all tensors which results from the main interaction axes (Kasir, 1993).

Using the expression describing the DIF, f_{dd} as given below (Graybeal, 1988).

$$f_{dd} = \frac{g_i g_j \beta^2}{h}(\bar{S}_i \cdot \underline{D} \cdot \bar{S}_j) \qquad (3)$$

Where:

$\underline{D}$ is the dipole coupling tensor, and for the case of identical spins, the tensor will have the following form:

$$\underline{D} = f_{\max}\begin{vmatrix} 3\ell^2-1 & 3\ell m & 3n\ell \\ 3\ell m & 3m^2-1 & 3mn \\ 3n\ell & 3mn & 3n^2-1 \end{vmatrix} \tag{4}$$

ℓ, m and n are the direction cosines of $\bar{r}_{ij}$. The magnitudes of the position vectors, the normalized maximum frequency $f_{\max}$ and the geometric parts of tensors for the six classes of ions are shown in Table (1) (Kasir, 1993).

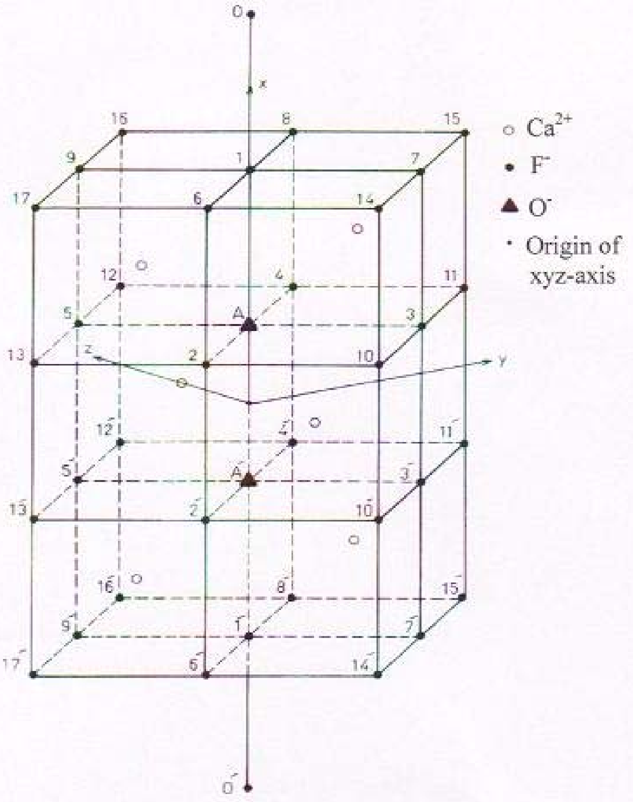

Fig 1: The postulated model for the oxygen center incorporated in CaF_2 crystal.

Table 1: r_{ij} , f_{max} and the geometric parts of tensors for the six classes.

	Class 1	**Class 2**	**Class 3**	**Class 4**	**Class 5**	**Class 6**
$r_{ij} \times 10^{-10}$ m	6.825	4.095	3.052	4.922	4.095	5.628
f_{max} MHz	0.2349	1.0876	2.6272	0.6263	1.0876	0.4189
D_{xx} MHz	0.4698	2.1752	-1.0509	0.6745	-0.7251	0.2464
D_{xy} MHz	0	0	2.2292	0.6131	1.0254	0.6259
D_{xz} MHz	0	0	2.2292	0.6131	0	0
D_{yx} MHz	0	0	2.2292	0.6131	1.0254	0.6259
D_{yy} MHz	-0.2349	-1.0876	0.5254	-0.3382	1.8127	0.1725
D_{yz} MHz	0	0	2.9425	0.2890	0	0
D_{zx} MHz	0	0	2.2292	0.6131	0	0
D_{zy} MHz	0	0	2.9425	0.2890	0	0
D_{zz} MHz	-0.2349	-1.0876	0.5254	-0.3382	-1.0876	-0.4189

When we apply an external magnetic field $\bar{B}$ along the c-axis of the crystal, the resonance frequency of each ions is displaced due to the effect of magnetic dipolar interaction. This displacement can be represented roughly in one dimension for a pair of like spins by the following simplified formula (Pool, 1971 ; Graybeal, 1988).

$$f_{dd} = \gamma B \pm f_{max}(3\cos^2\theta - 1)M \qquad (5)$$

Where each spin is quantized along the magnetic field $\bar{B}$, M is the projection of the spin along the principle c-axis of the crystal, γ is the magnetogyric ratio and θ is the angle between the vector $\bar{r}_{ij}$ and $\bar{B}$. In actuality, each vector with subscript index i characterize with the angle θ and Φ, as shown in Fig.2, but for simplicity only the azimuthal angle θ is shown in equation (5).

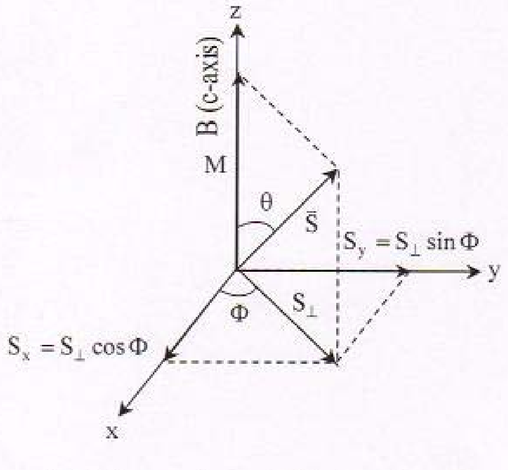

Fig. 2: The quantized spin $\bar{S}$ in three dimensions.

When applying magnetic field $\bar{B}$, a detailed geometrical calculations has been done to relate the angles done by the vector $\bar{B}$ and the x, y and z coordinates, for two different combinations of xyz system, with the angle α designated between $\bar{B}$ and the principle axis under consideration.

A computer program was employed to evaluate the tabulated parameters and study the magnetic field dependence of the DIF for the following two cases: (a) Rotation axis of $\bar{B}$ // [100] direction, i.e., the rotation axis of $\bar{B}$ // to the normal to the plane containing the vector $\bar{B}$ and passing through the origin of xyz coordinate system (in Fig. 3, the rotation axis is directed in the x-direction coordinate). And (b) rotation axis of $\bar{B}$ // [110] direction, i.e., the rotation axis of $\bar{B}$ // to the normal to the plane [110] containing the vector $\bar{B}$ and passing through the origin of xyz coordinate system (in Fig. 4, the rotation axis is directed in the y-direction coordinate).

The variation of DIF with magnetic field intensity B were analyzed in each case using one combination of coordination system xyz with the direction of $\bar{B}$ as shown in Fig.(3) and Fig.(4). In both cases, the variations of DIF with B have been analyzed for the four selected angles $\alpha = 0^\circ, 30^\circ, 60^\circ$ and 90°. These cases are illustrated in figures (5 to 16).

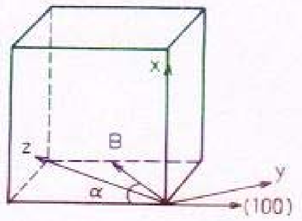

Fig. 3: Rotation axis of $\bar{B}$ // [100] direction i.e., in the x-direction coordinate.

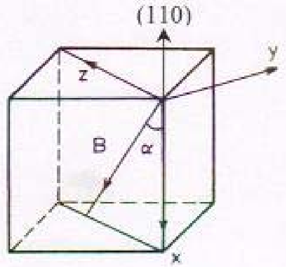

Fig. 4: Rotation axis of $\bar{B}$ // [110] direction i.e., in the y-direction coordinate.

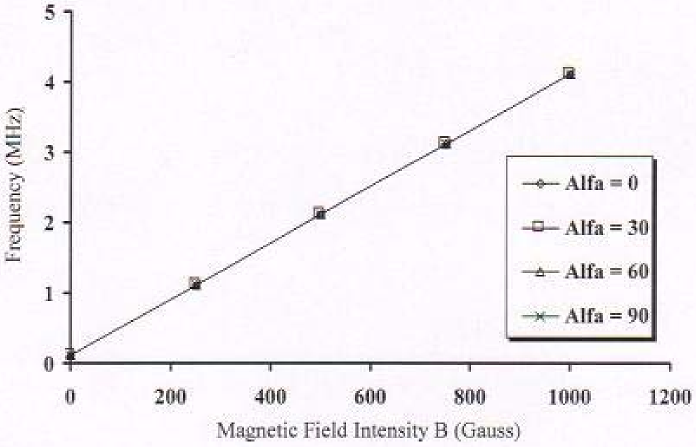

Fig 5: Magnetic field dependence of DIF of O$^-$ center in CaF$_2$, Rotation axis of $\bar{B}$ // [100], class 1 ions

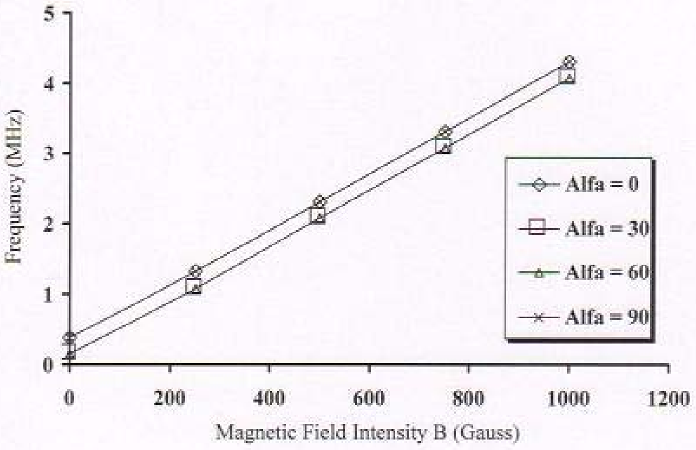

Fig 6: Magnetic field dependence of DIF of O$^-$ center in CaF$_2$. Rotation axis of $\bar{B}$ // [100], class 2 ions.

CONCLUSION

The figures indicate that the displacements in the resonance frequency due to the dipolar interactions are resulted in different values and signs for different angles, but at higher values of B, the displacements become positive and increase linearly with B.

Clearly, the magnetic dipolar interaction at low magnetic field intensity is more complex than given in equation (5) and in general we are dealing with tensor quantities. At higher magnetic field intensity, when B becomes greater than 1kG, all the dipoles are oriented parallel to $\vec{B}$ and the DIF becomes appreciably shifted in a linear form. The linear magnetic field variation of DIF for the different classes at higher magnetic field intensity ranged from 1kG up to 20kG with the exception of class 3, have approximately the same magnitude for the four values of α, i.e. $\frac{\Delta \nu}{\Delta B} = 0.004$ MHz/Gauss, while this quantity for class 3 is $\frac{\Delta \nu}{\Delta B} = 0.0038$ MHz/Gauss for the four values of α.

Figures 5 to 16 enable us to get benefits of using an external magnetic field in tuning an absorbing medium containing such oxygen centers to absorb a definite wavelength of interacting electromagnetic radiation. The special case shown by Fig.7, theoretically indicates that the ionic system of the oxygen ion centers has a resultant magnetic moment directed antiparallel to the applied magnetic field $\vec{B}$. For this reason, the interaction of this magnetic moment with $\vec{B}$ showed an effect of decreasing the dipolar interaction frequency at low external magnetic field intensities, but as $\vec{B}$ increased in magnitude, the resultant magnetic moment oriented parallel to $\vec{B}$ and the DIF started to increase in a non-linear form as a function of B. But at magnetic field intensities ranged from 1kG up to 20 kG and higher, the dependence of DIF on B followed a linear variation as mentioned before. Therefore, for applied work, one can get benefits in using such data in tuning experiments, by selecting a known point at the linear part of the graphs given in figures 5 to 16 and by the help of the magnitude of the slopes $\Delta \nu / \Delta B$ mentioned above for each case, the magnitude above for each case, the magnitude of $\vec{B}$ can be calculated to suit a desirable tuning frequency.

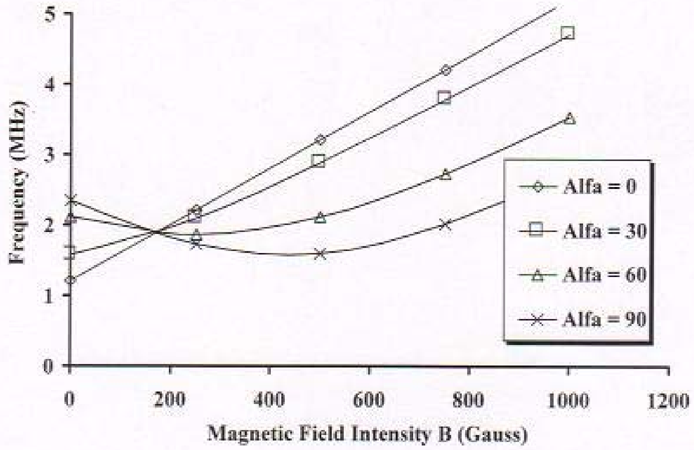

Fig 7: Magnetic field dependence of DIF of O⁻ center in CaF_2. Rotation axis of $\vec{B}$ // [100], class 3 ions.

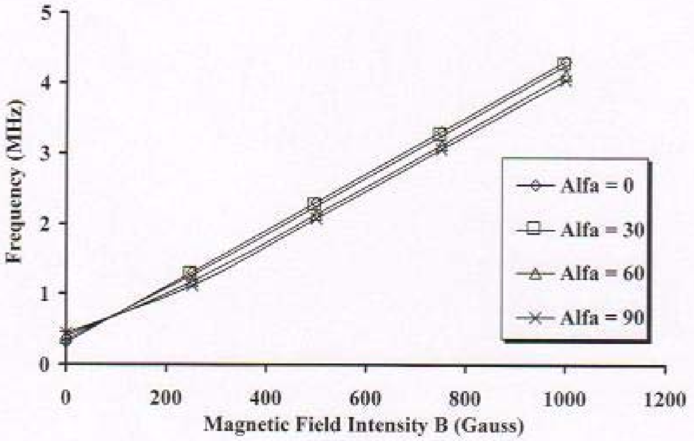

Fig 8: Magnetic field dependence of DIF of O⁻ center in CaF_2. Rotation axis of $\vec{B}$ // [100], class 4 ions

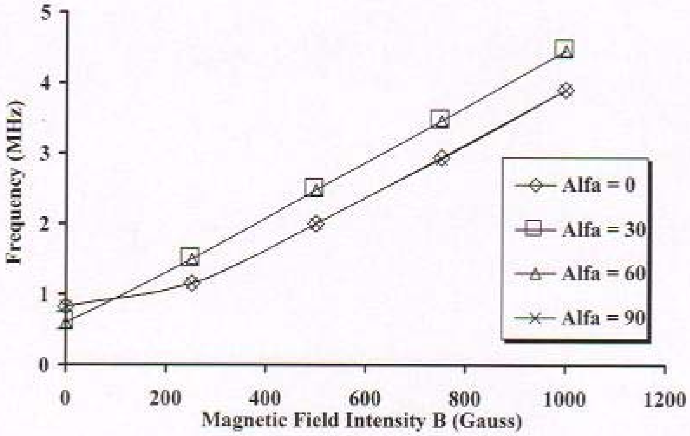

Fig 9: Magnetic field dependence of DIF of O⁻ center in CaF$_2$.
Rotation axis of $\bar{B}$ // [100], class 5 ions.

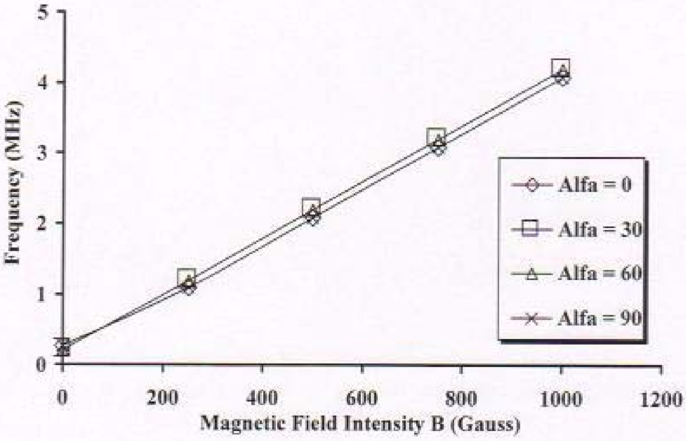

Fig 10: Magnetic field dependence of DIF of O⁻ center in CaF$_2$.
Rotation axis of $\bar{B}$ // [100], class 6 ions.

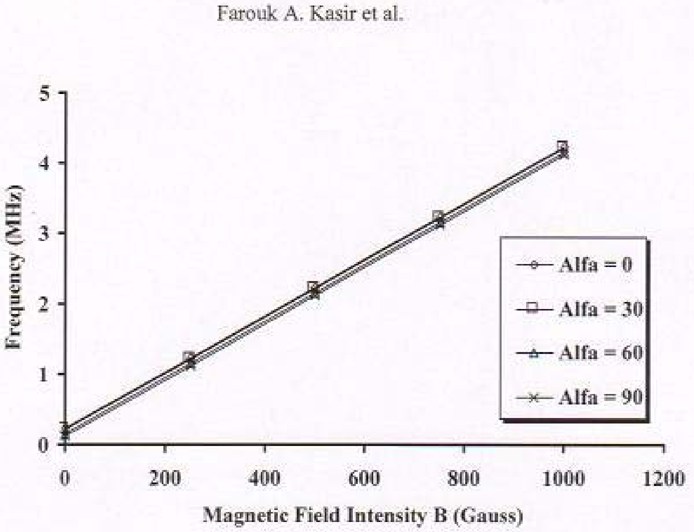

Fig 11: Magnetic field dependence of DIF of O^- center in CaF_2.
Rotation axis of $\vec{B}$ // [110], class 1 ions.

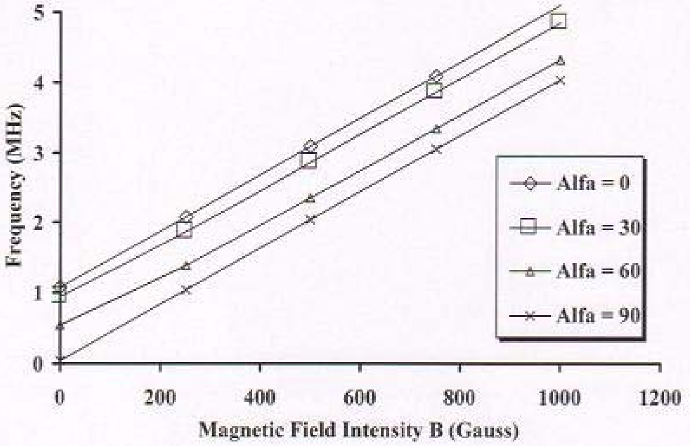

Fig 12: Magnetic field dependence of DIF of O^- center in CaF_2.
Rotation axis of $\vec{B}$ // [110], class 2 ions.

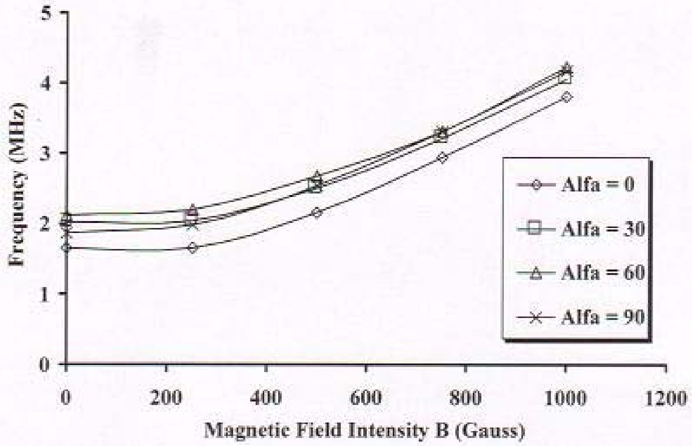

Fig 13: Magnetic field dependence of DIF of O^- center in CaF_2.
Rotation axis of $\bar{B}$ // [110], class 3 ions.

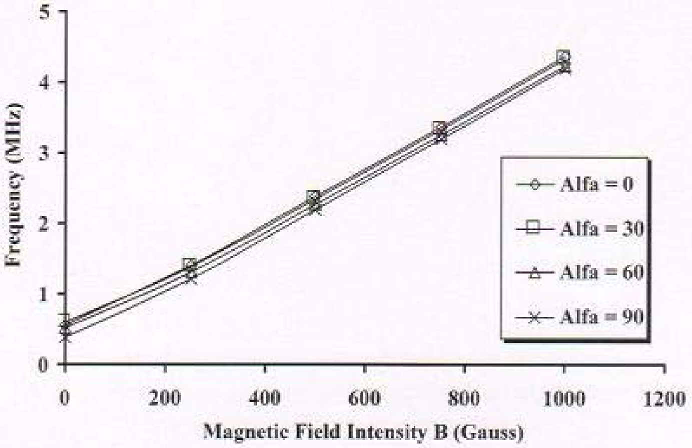

Fig 14: Magnetic field dependence of DIF of O^- center in CaF_2.
Rotation axis of $\bar{B}$ // [110], class 4 ions

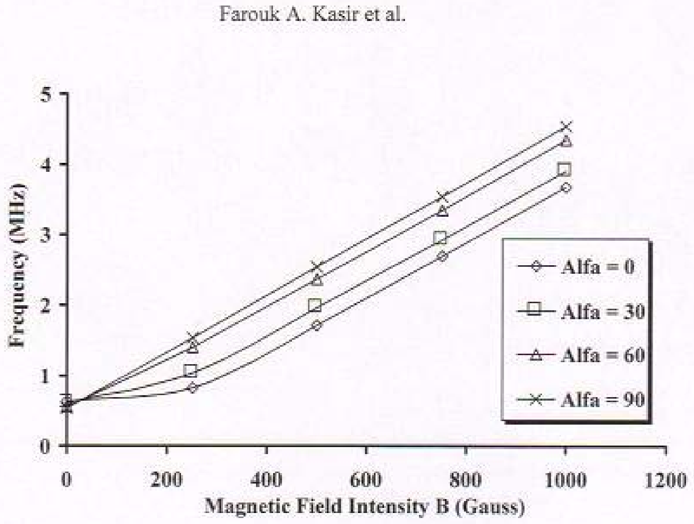

Fig 15: Magnetic field dependence of DIF of O^- center in CaF_2.
Rotation axis of $\vec{B}$ // [110], class 5 ions

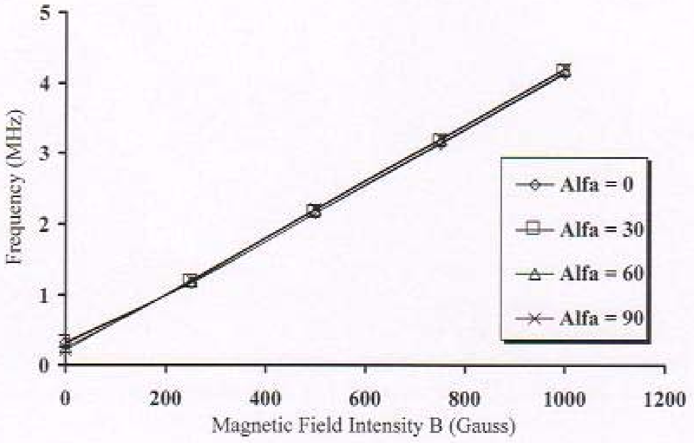

Fig 16: Magnetic field dependence of DIF of O^- center in CaF_2.
Rotation axis of $\vec{B}$ // [110], class 6 ions.

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