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# The search for an EFG equation of state in $ThM_3$ compounds (with M = Sn, In, Si, Ge, Ga, Rh, Pb, Tl)

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ABSTRACT

I have investigated the behavior of the electric field gradient (EFG) at M site in $ThM_3$ compounds (with M = Sn, In, Si, Ge, Ga, Rh, Pb, Tl) under pressure. I have found that the magnitude of EFG increases with pressure in all compounds. Furthermore I have shown that in $ThM_3$ (with M = In, Ga, Pb, Tl), this increase follows a common trend. Thereby I have reached an equation of state for the EFG in this group.



## 1. Introduction

All nuclei with a nuclear spin quantum number $I>1$ have a nonspherical nuclear charge distribution and an electric quadrupole moment $Q$. The nuclear quadrupole moments are often known only with limited accuracy and their determination is still an active field of research. The interaction between this quadrupole moment $Q$ and the electric field gradient (EFG) at an atomic site with noncubic point symmetry in a crystal can be measured by various methods, for example nuclear magnetic resonance (NMR), nuclear quadrupole resonance (NQR), or Mössbauer measurement, and is used for the characterization of surfaces, impurities, and vacancies [1,2]. From such experiments the amount of the electric hyperfine splitting, $\Delta E_{hf}$, can be obtained:

$$\Delta E_{hf} = f(I)eQq \tag{1}$$

where $q$ represents the EFG and $f(I)$ is a known function of the nuclear spin quantum number. Thus if $q$ is somehow known, a $\Delta E$ measurement determines $Q$, while if by an independent measurement the quadrupole moment $Q$ of the nucleus is known, a $\Delta E$ measurement can be used to determine $q$. EFG which may be calculated uniquely from the charge density, depends sensitively on the anisotropy of the charge density close to the nucleus; therefore, any redistribution of charge under pressure, is reflected on the EFG, so that the calculation of the EFG under pressure could be used to give insight to charge redistributions under pressure at any nuclei in the compound. In this paper I have investigated the effect of pressure on the EFG around the M nucleus in the presence of spin–orbit coupling for $ThM_3$ compounds (with M = Sn, In, Si, Ge, Ga, Rh, Pb, Tl). To the best of my knowledge, there are no experimental or theoretical reports on the pressure dependence of EFG for these compounds.

The EFG is a traceless, symmetrical tensor of rank 2, and is a measure of the deviation from spherical symmetry of the electronic charge density around the nucleus under consideration. In the principal axis, the EFG tensor is diagonal with diagonal elements $V_{xx}$, $V_{yy}$, $V_{zz}$ and $V_{xx}+V_{yy}+V_{zz}=0$. The principal axis is conventionally labeled such that $|V_{zz}|\geqslant|V_{yy}|\geqslant|V_{xx}|$. Instead of specifying two of the three diagonal elements, usually the couple $(V_{zz},\eta)$ is specified, where $\eta$ is called the asymmetry parameter which is equal to $(V_{xx}-V_{yy})/V_{zz}$. Therefore, one can only evaluate the main component of the EFG ($V_{zz}$) and the asymmetry parameter ($\eta$) to determine the two independent components of the EFG in the principal axis. In this paper the focus is only on the $V_{zz}$ as calculated electric field gradient, since the asymmetry

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parameter is zero in this case. Since a full potential without any restriction on its shape from the total charge density of the infinite system (including the nuclear charges) is calculated, the main component of EFG tensor is obtained directly form the $L = 2$, $M = 0$ component of potential expansion inside the spheres. The main component of the EFG tensor is calculated using the

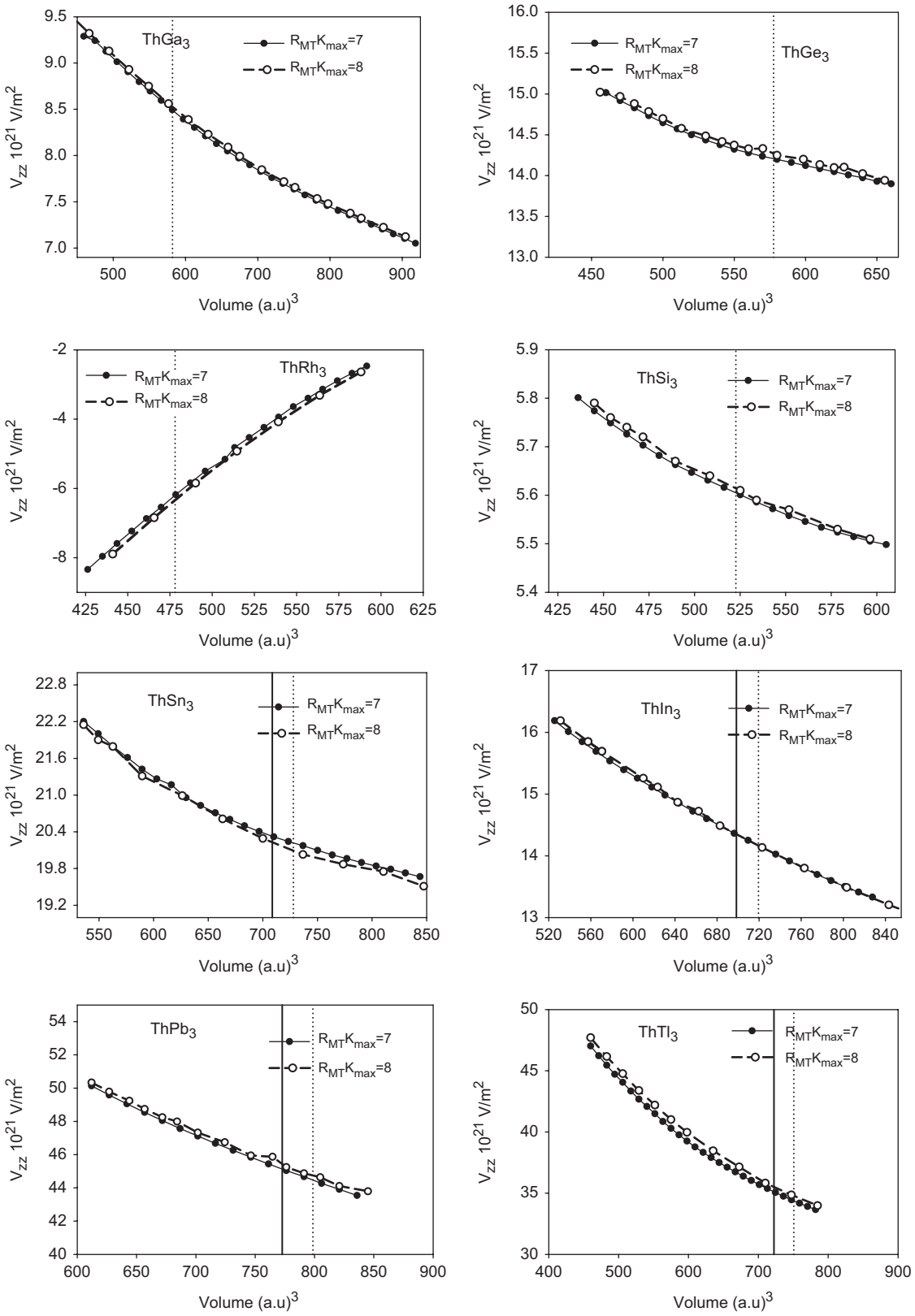


**Fig. 1.** $V_{zz}$ at M site in $ThM_3$ compounds as a function of the unit cell volume. The solid and dotted lines are the experimental and calculated equilibrium volume respectively.