Raman response of Stage-1 graphite intercalation compounds revisited

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We present a detailed in-situ Raman analysis of stage-1 KC₈, CaC₆, and LiC₆ graphite intercalation compounds (GIC) to unravel their intrinsic fingerprint. Four main components were found between 1200 cm⁻¹ and 1700 cm⁻¹, and each of them were assigned to a corresponding vibrational mode. From a detailed line shape analysis of the intrinsic Fano-lines of the G- and D-line response we precisely determine the position (ω_ph), line width (Γ_ph) and asymmetry (q) from each component. The comparison to the theoretical calculated line width and position of each component allow us to extract the electron-phonon coupling constant of these compounds. A coupling constant λ_ph < 0.06 was obtained. This highlights that Raman active modes alone are not sufficient to explain the superconductivity within the electron-phonon coupling mechanism in CaC₆ and KC₈.

I. INTRODUCTION

$\text{Sp}^2$ hybridized carbon allotropes have unique structural properties in different dimensions like graphite (3D), graphene (2D), single walled carbon nanotubes (1D), and fullerene molecules (“quasi 0D”). They have been widely studied due to their interesting electronic properties ranging from metallic, semimetallic, (zero gap) semiconducting to wide gap semiconducting and insulating [1–4]. One unique possibility to tailor their electronic properties is by intercalation of alkali and alkaline-earth ions. These intercalation compounds are particular appealing for their application in batteries and because of their superconducting phases. Superconductivity, as a result of alkali-metal intercalation, was first studied by Henning [5] in Graphite Intercalation Compounds (GIC) and further studies [6, 7]. However, until 1981, the critical temperature (T_c) in stage-1 XC₈ GIC (X=K, Rb, and Cs) reported was low [1], not higher than 0.135 K. The comparison to the theoretical calculated line width and position of each component allow us to extract the electron-phonon coupling constant of these compounds. A coupling constant λ_ph < 0.06 was obtained. This highlights that Raman active modes alone are not sufficient to explain the superconductivity within the electron-phonon coupling mechanism in CaC₆ and KC₈.

For GIC, the observation of superconductivity of CaC₆ in 2005 with a high T_c of 11.5 K [19] triggered further research in the field and led to alternative explanations of the superconducting electron phonon coupling. For instance, Kim et al. attribute superconductivity in CaC₆ to the high-energy C modes [20]. Hinks et al. [21] report that the low-energy modes of the intercalant were responsible for superconductivity inferred from specific heat analysis, while first principle calculations predicts equal coupling to both groups of phonons [9, 22]. Therefore, the exact contribution of the different coupling phonons still remain elusive.

Raman spectroscopy became then an important tool to determine the exact contribution of each phonon, and it opened a route for revealing the coupling mechanism in superconducting fullerides and GICs. Hence, it serves as a key tool to analyze the electron phonon coupling con-
stant (\(\lambda\)) from a renormalization of the optical response of the intra-molecular C_{60} modes and of the graphitic G-line response. Recent Raman studies on the G-line response of different stage-1 GIC reported the assignment of the electron phonon coupling (EPC) induced line width \(\gamma^{EPC}\) to the 1510 cm\(^{-1}\) mode \([23,24]\), which has been explained by the inclusion of non adiabatic phonon calculations \([24,26]\). However, the intrinsic G-line response in heavily doped graphite compounds are still elusive because of the influence of defects and laser induced deintercalation, as recently reported using a micro Raman analysis for CaC\(_6\) \([24]\) and for KC\(_8\) single crystals \([27]\).

In this contribution we report a detailed study of the D- and G-lines in KC\(_8\), CaC\(_6\), and LiC\(_6\) GIC, in order to unravel their intrinsic phonon components and its relation to the electron phonon coupling constant responsible for superconductivity. From the analysis of the optical phonons observed, we assign their role in the superconductivity coupling mechanism in comparison with previous results of electron doped GIC.

### II. EXPERIMENTAL, AND MEASUREMENT DETAILS

The synthesis of KC\(_8\) was performed in-situ under high vacuum (\(<4\times10^{-8}\) mbar) conditions in a quartz tube with natural graphite flake single crystals from different sources, and a potassium ingot with 99.95\% purity (Aldrich) for the intercalation. Potassium was evaporated until golden crystals were obtained. This phase can be directly assigned to stage-1 KC\(_8\) phase from a comparison of the Raman response with previous combined Raman and XRD results \([27,28]\). CaC\(_6\), and LiC\(_6\) were prepared in a sealed ampoule by using a procedure described elsewhere \([29]\). Highly oriented pyrolytic graphite (HOPG) flakes were degassed and used for lithium and calcium intercalation for 10 days under He atmosphere (ca. 0.5 atm). The ampoule was then opened in the glove box and gold colored product was extracted from the melt. Powder x-ray diffraction measurements were carried out using a Stadi-P diffractometer (CuK\(_\alpha\)) to confirm the intercalation stage in CaC\(_6\) and LiC\(_6\). For the Raman analysis every GIC was kept in vacuum (\(<4\times10^{-8}\) mbar) in order to avoid de-intercalation due to exposure to air. The Raman analysis, was performed with a HORIBA LabRam at room temperature, with a 568 nm wave length, and 0.25 mW of laser power. Every spectrum were acquired under the same conditions in a range from 500 cm\(^{-1}\) up to 2500 cm\(^{-1}\) and the line positions were calibrated by gauge lamps.

### III. RESULTS AND DISCUSSION

In the Raman response of stage-1 GIC eight optical vibrational modes are present \([28]\) in the following irreducible representation:

\[
\Gamma = 2A_{2u} + 2B_{2g} + 2E_{1u} + 2E_{2g}
\]

The \(E_{2g}\), and the \(E_{2g}\) vibrational modes are Raman active, and the \(A_{2u}\) and \(E_{1u}\) belong to infra-red active modes \([1,30]\). There are some other modes in graphite which are forbidden in perfect graphite and only become active in the presence of disorder like the mode with \(A_{1g}\) symmetry. In Fig. 1(a), the optical modes of graphite are depicted. Previous Raman studies in GIC have confirmed the presence of the \(E_{2g}\) mode around 1600 cm\(^{-1}\), the \(A_{2u}\) (c-axis mode) around 500 cm\(^{-1}\), and the absence of the \(A_{1g}\) \([1,28]\). The c-axis mode has being attributed to an out-of-plane C motion in graphite \([24]\). This mode correspond to the \(M\) point of the graphene Brillouin zone, and it becomes Raman active when high intercalation levels are achieved. In agreement with the literature, we observe (as shown in in Fig. 1(b)), that the c-axis mode is present solely in KC\(_8\) around \(<560\) cm\(^{-1}\). Surprisingly and in agreement with previous studies neither in CaC\(_6\), nor in LiC\(_6\) this mode is observed \([23,31]\).

Regarding the G-line response all these previous studies reported one G-line which has a strong Fano line shape due to the coupling and the interference with the conduction electrons. Taking a closer look on the lineshape of the G-line response in Fig. 1(b), one can easily see that more than one component is present, and a detailed line shape analysis is needed in order to unravel their intrinsic response and related electron phonon coupling of these stage-1 GIC. The line-shape analysis of the G-line is discussed in detail below.

![Graph](https://via.placeholder.com/150)

**FIG. 1.** a) Optical modes of graphite. b) Raman spectra from KC\(_8\), CaC\(_6\), and LiC\(_6\) taken with 568 nm laser at room temperature and low laser power of 0.25 mW.
A. Analysis of the intrinsic G-line response of 
Stage-1 GIC

The structure of the intercalation stages in graphitic compounds, has been studied and it is well understood from x-ray diffraction [28]. However, the intrinsic Raman response of stage-1 GIC is still complicated by laser induced de-intercalation from a local heating of the sample with different laser power densities [30]. In addition, other factors such as 3D intrinsic disorder of the crystal also strongly affect the Raman response in GIC. For example, a graphite single crystal doped to stage-1 will remain polycrystalline due to a non-homogeneous intercalation. This will limit the achievable doping in these GIC [24, 32].

Hence, the previous experimental and theoretical results on the Raman response of KC$_8$ and CaC$_6$ reported in the literature are not conclusive with respect to the G-line shape and position. In different studies a wide range of different G-line positions between $\sim$1400 cm$^{-1}$ and $\sim$1600 cm$^{-1}$ are reported: i.e. at $\sim$1500 cm$^{-1}$ [1], between 1400 cm$^{-1}$ and 1550 cm$^{-1}$ [28], 1534 cm$^{-1}$ [26], 1547 cm$^{-1}$ [20], 1420 cm$^{-1}$ and 1582 cm$^{-1}$ [33]. In more recent experiments for calcium GIC [24, 25], potassium doped graphene and graphite [27, 32], and later in Li-graphite [31], the strongest G-line phonon response is observed around 1510 cm$^{-1}$ when the sample has the best quality (lowest defect content) and highest intercalation.

In Fig. 2a) the D- to G-band region of pristine stage-1 intercalation compounds with K, Ca, and Li is depicted and clearly shows the presence of shoulders in the response, which indicate different components. Nevertheless, in order to compare with the previous studies [26, 30, 33] we first conducted a line-shape analysis of the G-line by using a single Breit Wigner Fano (BWF) function. This yields parameters which are in good agreement to those results, and confirms that our samples have the same high quality of a true stage-1 compound. This is further supported by the fact that the G-line assigned to stage-2 compounds around 1600 cm$^{-1}$ is only increased upon e.g. laser induced de-intercalation (see Fig. 2 b).

In a second step a detailed and accurate analysis of the line-shape in the D- to G-band region of these GIC was conducted using four components. The assignment of each component to the A$_{1g}$ (D), E$_{2g}$, E$_{2g}$, modes, and the G-line of the stage-2 compound is explained in the following.

Regarding the line-shape, all components have been fitted using BWF functions of the form:

$$I(w) = I_0 \left(1 + \frac{w - \omega_{ph}}{\Gamma q^{1/2}} \right)^2 + A$$

where $\omega_{ph}$ is the phonon frequency, $\Gamma$ the line width or damping, $q$ the asymmetry parameter and $A$ an offset. For the first and fourth peak (D, and G), the asymmetry was $q=10^5$ approaching a Lorentzian function, while the second and third (splitted G-line) have a pronounced Fano interference. In the analysis, in order to get comparable results for each GIC, the same values of $\Gamma$, and
q were used to fit each respective component. The parameters are summarized in Table I together with the calculated values from the adiabatic and non-adiabatic phonons from Ref. 26.

The first mode observed in Fig. 2 a) between 1260 and 1360 cm$^{-1}$ has been previously attributed to particle size effects and/or the presence of disorder. It has been assigned to the $A_{1g}$ vibration, which is forbidden in perfect graphite. Therefore, this mode is called D-line (intrinsic “defect mediated”), and it involves the contribution from the phonons near the K zone boundary with a Lorentzian line-shape.

The second and third modes observed are assigned to the $E_{2g}$ graphitic mode of heavily doped graphene layers (Fig. 2 a). Both components have a pronounced asymmetry and they are well described by a BWF line-shape. We label the two modes as $E_{2g1}$ and $E_{2g2}$. The $E_{2g1}$ mode is located between 1528 cm$^{-1}$ and 1585 cm$^{-1}$ and it is attributed to not homogeneous or incomplete intercalation in stage-1 compounds. The $E_{2g2}$ mode locates at 1510 cm$^{-1}$ for KC$_8$ and CaC$_6$, and 1546 cm$^{-1}$ for LiC$_6$. It has a clear and strong Fano behavior which is characteristic of the fingerprint of stage-1 graphite intercalation compounds [24, 27]. When de-intercalation was induced in the samples, a decrease of these $E_{2g}$ modes was remarkably observed (see Fig. 2 b).

The fourth mode related to the G-line of their respective stage-2 compound is observed at 1612 cm$^{-1}$ for KC$_8$, 1600 cm$^{-1}$ for LiC$_6$, and at 1560 cm$^{-1}$ for CaC$_6$. The surprising low frequency in the case of CaC$_6$ was also found in Ref. 29 and explained as a de-intercalated phase in CaC$_6$. As mentioned above, the increase of this fourth component is highlighted in the partly de-intercalated stage-1 compounds in Fig. 2 b), and points towards a phase separation upon de-intercalation.

B. Analysis of the Electron-Phonon Coupling

The previous results are very important for the correct determination of the stage, and electron-phonon coupling constant $\lambda_{ph}$ responsible for superconductivity within the BCS theory [24, 29, 30]. This constant is directly related to the intrinsic G-line phonon frequency, and to the adiabatic ($\omega_A$) and non-adiabatic ($\omega_{NA}$) phonon frequencies. Saitta et al. [26] have analyzed the EPC in many different stage-1 GIC from a difference in the experimental phonon frequency to the calculated phonon frequency in the adiabatic and non-adiabatic limit. In order to determine the electron phonon scattering renormalized line width $\gamma_{EPC}$ [24, 26] we used:

$$\frac{\gamma_{EPC}}{2} = \sqrt{(\omega_{ph} - \omega_A)(\omega_{NA} - \omega_{ph})}$$  \hspace{1cm} (1)

We obtain $\gamma_{EPC}$ values for KC$_8$, CaC$_6$, and LiC$_6$, which are in very good agreement to our experimental $\Gamma_{ph}$ value obtained from our BWF fit, Table II. In Fig. 3 we show the location of our $\gamma_{EPC}$ with respect to the expected linear tendency to $\Gamma_{ph}$ as predicted by Saitta et al. [26]. It is important to notice that some components of the G-line in KC$_8$, CaC$_6$, and LiC$_6$ bring a $\gamma_{EPC} = 0$, which means that they do not show the non-adiabatic effects for layered metals and therefore they do not contribute to the electron-phonon coupling constant $\lambda_{ph}$. In comparison to the experimental $\Gamma_{exp}$ and $\gamma_{EPC}$ from Ref. [25, 26, 38] (Fig. 3), our results using the $E_{2g2}$ mode are in better agreement to the linear trend expected for $\Gamma \approx \gamma_{EPC}$. This confirms the importance of every optical mode in the range between the adiabatic and non-adiabatic frequency range ($\omega_A$-$\omega_{NA}$), and confirms that the $E_{2g2}$ component is the intrinsic stage-1 vibrational mode with the strongest non-adiabatic effect on the EPC.

We now turn to a detailed analysis of the EPC constant $\lambda_{ph}$. Different values have been already reported and used to calculate the critical temperature of KC$_8$, CaC$_6$, and LiC$_6$ with values around 5 K, 11.5 K, and 0.9 K, respectively, in agreement with some experimental and theoretical studies [8, 40]. In order to extract $\lambda_{ph}$ from the phonon line-width ($\Gamma$) and position ($\omega_{ph}$) from our Raman data we used [41]:

$$\lambda_{\Gamma,K} = \frac{A_{uc} F^2_{\Gamma,K}}{2 M \omega_{\Gamma,K} v_F^2}$$ \hspace{1cm} (2)

where the electron-phonon coupling strength is given by $D_{exp}$:

$$\Delta \Gamma_G = \frac{A_{uc} D^2_{exp}}{8 M v_F^2}$$ \hspace{1cm} (3)

and $A_{uc}$ is defined as the area of the graphene unit cell, $M$ is the carbon atom mass, $v_F$ is the Fermi velocity, $\Delta \Gamma_G$ is the Landau damping phonon decay rate given by
\[ \Delta \Gamma_G = \Gamma_{ph} - \Gamma_{Graphite}, \text{ and } F^2_{\Gamma K} \text{ has dimensionality of a force taking in consideration the lattice displacement along the corresponding optical phonon mode. By using Eq. 2 and the definition of } F^2_{\Gamma K} = 4(D^2_{\Gamma K} F), \text{ and } F^2_{\Gamma K} = 2(D^2_{\Gamma K} F) \text{ from Ref. } [29, 41] \text{ we calculate the values for } \lambda_{\Gamma K} \text{ for each phonon in the } \Gamma-K \text{ branch observed in the G-line region as summarized in the right column of Table II. } \langle D^2_{\Gamma K} \rangle \text{ were taken from the DFT\textit{GGA} calculations in Graphite [39] as they are closer to our electron-phonon coupling strength } (D_{exp}). \]

By using the averaged electron-phonon coupling constant \( \lambda_{ph} = \lambda_{\Gamma} + \lambda_{K}, \text{ and the position } \omega_{ph} \text{ from the strongest optical mode in } KC_8, \text{ CaC}_6, \text{ and LiC}_6 \text{ one can estimate the critical temperature } T_c \text{ using McMillan’s formula [42]. Taking our } \omega_{ph} \text{ values converted in to phonon temperature } \Theta, \mu^* \approx 0.14 \text{ from [43], and } \lambda_{ph} \text{ from the Raman analysis, we obtain } \lambda_{ph} < 0.06 \text{ values, which are too low to explain superconductivity within EPC mechanism using these high-frequency Raman active modes.} \]

However, this is not a general behavior in intercalation compounds. Electron-phonon studies in alkali-intercalated fullerenes showed the possibility to attribute the strongest \( \lambda_{ph} \text{ contribution for superconductivity to the } \text{Hg(1) mode in } \text{AsC}_6 \text{ fullerides [13, 14]. More over, in agreement to the analysis reported by Yao et al. in Ref. [10] our } D_{exp} \text{ presented the same trend as the one observed in fullerides intercalation compounds. Therefore, we can confirm that the larger the value of } 1/q, \text{ the weaker the coupling strength } D_{exp} \text{ in GIC and fullerides.} \]

On the other hand, in comparison to the EPC constant \( \lambda_{RePC} \) reported using an analysis of the self energy results in ARPES [8, 44], our \( \lambda_{ph} \text{ values are about a factor of 10-15 lower. Since, in the case of } CaC_6 \text{ superconductivity was confirmed at } T_c=11.5 \text{ K, only the } \lambda_{RePC} \text{ would be sufficient to explain this high superconducting transition temperature. Hence, the low } \lambda_{ph} \text{ proves that optical modes from the G-line in } stage-I \text{ GIC are not sufficient to explain } T_c \text{ in the electron-phonon driven superconducting coupling mechanism and additional not optically active modes might play an important role.} \]

IV. CONCLUSIONS

We have performed a detailed in situ Raman study of the most common GIC (\( KC_8, CaC_6, \text{ and LiC}_6 \)). We identify four main peaks in the D- to G-band region, and all these Raman responses match the spread of different line shapes reported in the literatures so far. From an examination of the fine structure in the G-line response we assign each peak to their corresponding vibrational mode and phonon branch.

We found the strongest Fano behavior of the G-line at 1510 cm\(^{-1}\) in \( KC_8 \text{ and CaC}_6, \text{ not like in } \text{LiC}_6, \text{ which highlights the importance of this mode to the superconductivity coupling mechanism within the BSC theory, and confirms the importance of this } E_{2g} \text{ mode to nonadiabatic effects. By using this mode, we obtain a very good agreement to the theoretical predicted line-width } \gamma_{EPC} \approx \Gamma_{ph} \text{ especially for } CaC_6. \]

Finally, we find a very small EPC \( \lambda_{ph} < 0.06 \text{ which is much too low to explain the high } T_c \text{ in this graphite}

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
\multicolumn{7}{|c|}{Table II. Electron-phonon coupling parameters from the G-line Raman analysis. The values of } \omega_{ph}, \Gamma_{ph}, \gamma_{EPC} \text{ are in cm}^{-1} \text{ and they were extracted from the BWF analysis of the Raman spectrum. } D_{exp} \text{ is the electron-phonon coupling strength from Eq. 3 in (eV/Å).} \\
\hline
\text{GIC} & \omega_{ph} & \Gamma_{ph} & \gamma_{EPC} & \gamma_{EPCa} & D_{exp} & OB^b & \lambda_{GIC} \gamma_{EPC}^c \\
\hline
\text{KC}_8 & 1274 & 24.3 & 230 & - & 14 & K & 0.0247 \\
\text{CaC}_6 & 1510 & 125.6 & 163 & 157 & 51 & G & 0.0200 \\
\text{LiC}_6 & 1547 & 70.9 & 0 & - & 36 & G & 0.044 \\
\hline
\text{KC}_8 & 1585 & 70.9 & 34 & 36 & 36 & G & 0.0199 \\
\hline
\text{CaC}_6 & 1525 & 71.0 & 68 & 68 & 36 & G & 0.0222 \\
\text{LiC}_6 & 1510 & 70.9 & 34 & 36 & 36 & G & 0.0199 \\
\hline
\end{tabular}
\end{table}
intercalated compounds. This points out that, other phonons including acoustic modes and other electronic states might play an important role in explaining the superconducting pairing in GIC.

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