Raman scattering study of spin-density-wave-induced anisotropic electronic properties in \( \text{AFe}_2\text{As}_2 \) \((A = \text{Ca, Eu})\)

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We present a polarization-resolved and temperature-dependent Raman scattering study of \( \text{AFe}_2\text{As}_2 \) \((A = \text{Ca, Eu})\). In the spin-density-wave phase, spectral weight redistribution is observed in the fully symmetric and non-symmetric scattering channels at different energies. An anisotropic Raman response is observed in the fully symmetric channel in spontaneously detwinned \( \text{CaFe}_2\text{As}_2 \) samples. We calculate the orbital-resolved electronic structures using a combination of density functional theory and dynamical mean field theory. We identify the electronic transitions corresponding to these two spectral features and find that the anisotropic Raman response originates from the lifted degeneracy of the \( d_{xz/yz} \) orbitals in the broken-symmetry phase.

The parent and underdoped compounds of the 122 family \((\text{AFe}_2\text{As}_2)\) of iron-pnictide superconductors harbor an antiferromagnetic ground state with a collinear stripe spin order of Fe ions. The formation of a spin-density-wave (SDW) order at a temperature \( T_{SDW} \) is accompanied by a tetragonal to orthorhombic structural distortion in which the \( C_4 \) rotational symmetry is broken. Although the lattice distortion is small, the electronic anisotropy can be large. For a strain-free sample, a twin domain structure with a typical dimension of a few micrometers usually forms with orthogonally aligned antiferromagnetic directions. In many macroscopic symmetry-sensitive experiments, the response along the antiferromagnetic and ferromagnetic directions can be mixed and averaged. However, strongly anisotropic responses in the dc and ac electrical conductivity, the thermoelectric power, and the magnetic susceptibility along the two orthogonal directions, as well as in the on-site energy splitting of the \( d_{xz} \) and \( d_{yz} \) orbitals, have been reported for samples completely or partially detwinned following the application of a uniaxial strain or stress, or an in-plane magnetic field.

Electronic Raman scattering is an inelastic light scattering process that traces the density-density correlation function driven by the incident and scattered lights. With a proper choice of light polarization, it can separate states or collective excitations associated with certain symmetries belonging to the irreducible representations for the point group of a particular crystal. For example, the \( d \)-wave superconducting gap in cuprates results in a \( \omega \) Raman response in the nodal direction and a linear Raman response in the anti-nodal direction. In the iron-pnictides, the nematic fluctuations of the XY symmetry are observed in the tetragonal phase with cross-polarized light along the Fe-As directions. Therefore, it is of interest to study the Raman response for excitations of different symmetries across the structural and magnetic phase transitions.

In this paper, we present polarization-resolved electronic Raman measurements of the iron-pnictide parent compound \( \text{AFe}_2\text{As}_2 \) \((A = \text{Ca, Eu})\). We observe two spectral features with different symmetries below \( T_{SDW} \). One feature is a coherence peak in the fully symmetric channel that was previously assigned to the formation of a SDW gap near the \( M(\pi/a, 0, 0) \) point. Using symmetry analysis of a detwinned sample, as well as a combination of density functional theory and dynamical mean field theory (DFT+DMFT) calculations above and below \( T_{SDW} \), we show that this feature is an intra-orbital transition near the \( Z(0, 0, 2\pi/c) \) point. In the non-symmetric channel, we identify an additional small peak at lower frequency that originates from the lifted degeneracy of the \( d_{xz} \) and \( d_{yz} \) orbital at the \( \Gamma \) point.

The \( \text{CaFe}_2\text{As}_2 \) and \( \text{EuFe}_2\text{As}_2 \) samples employed in this study have been synthesized by Sn and Fe-As flux methods described in Refs.\(^{23,24}\). \( \text{CaFe}_2\text{As}_2 \) goes through a second-order phase transition at 170 K whereas \( \text{EuFe}_2\text{As}_2 \) goes through a first-order phase transition at 175 K. The high-temperature tetragonal structure belongs to the space group \( I4/mmm \) (point group \( D_{4h} \)) and the low-temperature orthorhombic structure belongs to the space group \( Fmmm \) (point group \( D_{2h} \)). Freshly cleaved \( \text{CaFe}_2\text{As}_2 \) and \( \text{EuFe}_2\text{As}_2 \) single crystals have been measured in a quasi-back-scattering geometry from the \( ab \) surface. The 476- and 647-nm laser beams of a Kr\(^+\) ion laser with a total incident power smaller than 15 mW were focused to a \( 50 \times 125 \) \( \mu \text{m}^2 \) spot on the sample surface. The scattered light was analyzed by a triple grating spectrometer and collected by a liquid \( \text{N}_2 \)-cooled CCD detector. The data were corrected for the spectral
response of the system at different wavelengths. The polarization configuration (e^x e^y) is defined by the polarization of the incident and scattered photons, e^x and e^y, respectively. The polarization vectors x = [110] and y = [110] are along the nearest Fe-Fe bonds corresponding, respectively, to the antiferromagnetic (AFM) and ferromagnetic (FM) directions in the SDW phase, and X = [100] and Y = [010] form a 45° angle with them.

In Fig. 1, we show the Raman response of CaFe_2As_2 and EuFe_2As_2 for the XY scattering geometry at various temperatures above and below T_{SDW}. We observe a spectral weight transfer from low frequency to above 800 cm^{-1} with the development of a coherence peak. As indicated in Figs. 1(c) and 1(d), the coherence peak in CaFe_2As_2 (EuFe_2As_2) hardens from 920 (800) to 1220 (1060) cm^{-1} from T_{SDW} to the lowest measured temperature. This spectral feature was previously assigned to the formation of a SDW gap, which is accompanied by the appearance of a Dirac cone in the electronic structure.

We performed polarization-dependent measurements on CaFe_2As_2 and EuFe_2As_2 samples. The electronic states in the vicinity of the Fermi level (E_F) in the iron-pnictides consists mainly of Fe 3d orbitals. Locally, these states decompose into A_{1g} (d_{z^2}), B_{2g} (d_{x^2−y^2}), B_{1g} (d_{xy}), and two E_{g} (d_{xz}, d_{yz}) states, which behave differently under the symmetry operations of the D_{4h} group. We note that in the low-temperature SDW phase the crystal structure of AFe_2As_2 is lowered to the D_{4h} group and the irreducible representations change. For example, A_{1g}(D_{4h}) and B_{2g}(D_{4h}) merge into A_{g}(D_{2h}), and A_{2g}(D_{4h}) and B_{1g}(D_{4h}) merge into B_{1g}(D_{2h}). We list all in-plane polarization configurations and the symmetry channels they can couple to in both the paramagnetic and SDW phases in Table I, from which the evolution of the D_{4h} and D_{2h} irreducible representations are directly shown.

Our results are displayed in Fig. 2. We first discuss the Raman responses obtained on CaFe_2As_2 (first row in Fig. 2). At room temperature, we observe that a continuum extends to the highest measured frequency in all polarization configurations. Typically, a twinned orthorhombic structure forms upon cooling down the samples below T_{SDW}, as can be viewed under a microscope with crossed-polarized light. To maximize the size of the domains, our samples were cooled down in two steps. At temperatures way above T_{SDW}, the samples were cooled at a rate...
paramagnetic state in the paramagnetic phase (i) and (j)) and SDW phase (k)-(n) along high-symmetry lines in the orbitals in high-symmetry points Γ and M in the momentum space. Filled and empty lobes represent the sign of the wave functions. The dashed blue lines show the four-Fe unit cell in the SDW phase. The dashed black lines are the xx or yz mirror planes. The black arrows represent the local moment in the SDW phase. A complete schematic of wave function phase change of the three dominant phases.

![Diagram of the $d_{xy}$ and $d_{yz}$ orbitals.](image)

**FIG. 3.** (Color online) (a) Diagram of the $d_{xy}$ and $d_{yz}$ orbitals. (b) High-temperature 2-Fe BZ (gray shade) and low-temperature folded BZ (dashed line). (c-h) Schematic representations of Fe $3d_{xy}$, $d_{xz}$, and $d_{yz}$ orbitals in real space at the high-symmetry points Γ and M in the momentum space. Filled and empty lobes represent the sign of the wave functions. The dashed blue lines show the four-Fe unit cell in the SDW phase. The dashed black lines are the xx or yz mirror planes. The black arrows represent the local moment in the SDW phase. A complete schematic of wave function phase change of the three dominant phases.

### TABLE I. Light polarization configurations and corresponding symmetry channels probed in the paramagnetic and SDW phases.

| Pol. | Paramagnetic | SDW |
|------|--------------|-----|
| XX   | $A_{1g} + B_{2g}$ | $A_{g} + B_{1g}$ |
| $A_{2g} + B_{2g}$ | Not a proper geometry |
| $A_{1g} + B_{2g}$ | $A_{g}$ |
| $A_{2g} + B_{1g}$ | $B_{1g}$ |

higher than 60 K/hr. Upon approaching $T_{SDW}$, though, this cooling rate was decreased below 1 K/hr. Using this procedure, a mono-domain in millimeter size formed in our CaFe$_2$As$_2$ samples, which we confirmed using laser illumination with XY polarization. In Figs. 2(a1)-(a4) we show the Raman scattering intensity of a CaFe$_2$As$_2$ sample slowly cooled down. The coherence peak around 1220 cm$^{-1}$ only appears in the XY, xx, and yy polarizations at low temperature. Moreover, a large anisotropy of intensity for this coherence peak is observed between the xx and yy polarizations, even though they share the same low-frequency phonon spectra and high-frequency response. Indeed, the intensity of the peak in the yy polarization is less than half of that in the xx polarization, and the frequency is slightly higher. In addition, for the XX and xy polarizations, we distinguish clearly a smaller feature at 830 cm$^{-1}$ that has not been reported in previous Raman studies.

We now switch to our results on EuFe$_2$As$_2$. Although we did not succeed in detwining completely the sample using the same cooling procedure, similar physics is observed. The paramagnetic state spectra in the XX and XY configurations are very similar to those obtained on CaFe$_2$As$_2$. As with CaFe$_2$As$_2$, a strong coherence peak is also detected in EuFe$_2$As$_2$ under the XY and xx (or yy) configurations, albeit for a slightly smaller peak frequency (1060 cm$^{-1}$). In order to confirm the Raman na-
ture of the features observed, we measured Raman spectra on the same sample using a 476-nm laser excitation. The results, displayed in Figs. 2(c1)-2(c4), show different backgrounds as compared to the ones recorded with 647-nm light. In particular, the broad peaks found at 1800 and 3200 cm$^{-1}$ in the 647-nm spectra are absent in the 476-nm spectra, suggesting that they possibly correspond to luminescence signals. Interestingly, the smaller feature found in CaFe$_2$As$_2$ using the $XX$ and $xy$ polarizations is only present under 476-nm excitation.

In order to understand the origin of these electronic Raman excitations, we calculated the band dispersion of CaFe$_2$As$_2$ by using DFT+DMFT in the paramagnetic and SDW phases$^{28}$. We used the experimental lattice constants and internal coordinates of the paramagnetic phase. The Coulomb interaction and the Hund’s coupling constants and internal coordinates of the paramagnetic phase. The Coulomb interaction and the Hund’s coupling are from Ref.$^{29}$. The band dispersions [single-particle spectral function $A(k, \omega)$] along high-symmetry lines are shown in Figs. 3(i)-(n) with the orbital characters represented by different colors. The high-symmetry points are labeled in Fig. 3(b).

The presence of different gap energies in two different symmetry channels in the SDW phase arises from the complexity of the folded band structures. The band structure near $E_F$ is dominated by the $d_{xx}$, $d_{xz}$ and $d_{yz}$ orbitals of Fe. In the high-temperature phase, there are three hole FSs around the $\Gamma$ point and two electron FSs around the M point. There is a SDW order that not only causes the lifting of the degenerated $d_{xz,yz}$ bands but also induces Brillouin-zone (BZ) folding from $A(\pi/a, 0, 2\pi/c)$ to $\Gamma$. At the $M$ ($M'$) point, the two electron bands hybridize with the three folded hole bands from $Z$ ($\Gamma$) and a band gap is opened around $M$ ($Z$). In contrast to the Dirac node at $E_F$ reported in BaFe$_2$As$_2$,$^{26,27}$, the Dirac point in CaFe$_2$As$_2$ is 45 meV above $E_F$. Interestingly, there is a second Dirac point at $E_F$ along the FM direction in the $k_z = 0$ plane between the $d_{yz}$ band and the folded $d_{xz}$ band. In the $k_z = 2\pi/c$ plane, the second Dirac cone carries the $d_{xz}$ characters and its energy is 36 meV below $E_F$.

Raman scattering is a small $q$ process since the momentum conservation requires the momentum transfer between the initial and final states to be equal to the momentum difference of the scattered and incident lights. As with infrared absorption, the interband electronic Raman scattering intensity is determined by the joint density of states and the coherence factor. In the case of non-resonance scattering, the scattering intensity is a reflection of the density of states of the initial and final states.

The symmetries of the Fe orbitals are derived from the symmetries of their wave functions. Away from the $\Gamma$ point, the phase term $e^{ik \cdot R}$ in the wave functions can change the parity of some bands$^{30}$. For example, we illustrate in Figs. 3(c)-(h) the $d_{x'y'}^{-}$, $d_{x'x'}^-$, and $d_{y'y'}^+$ orbitals at the $\Gamma$ and M point. At the $M$ point, the parity to the $yz$ mirror plane is the same as at the $\Gamma$ point, and the parity to the $xz$ mirror plane becomes the opposite.

We summarize the symmetry of the three dominant orbitals in the paramagnetic and SDW phases in Table I. A complete symmetry analysis is shown in the Appendix.

The selection rules between these orbitals are determined by the product of the initial-and-final-state symmetries. For the high-temperature paramagnetic phase, only the intra-orbital transitions are allowed in the $A_{1g}$ symmetry channel, while for the SDW phase, besides the intra-orbital transitions in the $A_{1g}$ symmetry channel, the $d_{xx}^+ \leftrightarrow d_{xx}^-$ and $d_{yz}^+ \leftrightarrow d_{xz}^-$ transitions become Raman active in the $B_{1g}$ symmetry channel. The selection rules for each in-plane symmetry channel in both the paramagnetic and SDW phases are listed in Table I. The Raman scattering vertices in the $B_{1g}$ and $B_{2g}$ symmetries for the one-Fe BZ for each pair of the orbital characters of the initial and final states are calculated in$^{31}$.

While phononic Raman scattering requires as a general selection rule that the symmetry of the phonon states be chosen by the incident and scattered light polarizations, electronic Raman scattering requires more complex selection rules for the symmetry of the initial and final states. The light polarized along the AFM direction $(x)$ can excite $d_{xx}$ bands. For light polarized along the FM $(y)$ direction, only $d_{yy}$ can be excited. Therefore, the peak in the $xx$ polarization can only arise from $d_{xx} \leftrightarrow d_{xz}$ transitions. Our calculations further confirm that the $A_{1g}$ symmetry excitation primarily comes from the $Z$ point, where a band gap opens between the original and the folded $d_{xz}$ bands (Fig. 3(i)).

![FIG. 4. (Color online) (a) $d_{xx} \leftrightarrow d_{yy}$ transition at the BZ center and $k_F$. The excitations are allowed in the shaded areas. (b) and (c) Differential Raman spectra between 300 and 24 K (50 K) in CaFe$_2$As$_2$ and EuFe$_2$As$_2$, respectively. The peak in (b) and (c), denoted by arrows, correspond to the excitations at the momentum indicated by arrows in (a).](image-url)
TABLE II. Symmetries of $d_{xy}$, $d_{yz}$ and $d_{xz}$ orbitals at high-symmetry momentum space points, and the allowed transitions in each symmetry channel in the paramagnetic and SDW phases.

| Momentum/orbitals | High-temperature paramagnetic phase, $D_{3h}$ | Low-temperature SDW phase, $D_{2h}$ |
|-------------------|-----------------------------------------------|-------------------------------------|
| $\Gamma$          | $B_{2g}$ $A_{1u}$ $E_g$ $E_u$ $E_g$ $E_u$    | $B_{1g}$ $B_{3g}$ $B_{1u}$ $B_{2g}$ $B_{2u}$ |
| $M$               | $E_u$ $E_g$ $A_{2u}$ $A_{2g}$ $A_{1u}$ $A_{1g}$ | $B_{3u}$ $B_{3g}$ $B_{1u}$ $B_{1g}$ $A_u$ $A_g$ |
| $M'$              | $E_g$ $E_u$ $A_{2g}$ $A_{2u}$ $A_{1g}$ $A_{1u}$ | $B_{3g}$ $B_{3u}$ $B_{1g}$ $B_{1u}$ $A_g$ $A_u$ |

Symmetry channel allowed transitions

| A$_1g$       | intra-orbital | |
| B$_{1g}$     | $d_{x^2}^+ \leftrightarrow d_{yz}^+$, $d_{xz}^+ \leftrightarrow d_{yz}^-$ |
| B$_{2g}$     | -             | |

| A$_g$        | intra-orbital | |
| B$_{1g}$     | $d_{x^2}^+ \leftrightarrow d_{yz}^+$, $d_{xz}^+ \leftrightarrow d_{yz}^-$ |

In conclusion, we reported temperature-dependent and polarization-resolved Raman scattering on twinned CaFe$_2$As$_2$ and EuFe$_2$As$_2$ and detwinned mono-domain CaFe$_2$As$_2$ single crystals. Two spectral features are observed in two different symmetry channels in the SDW phase. Based on symmetry arguments and DFT+DMFT calculations of the orbital-resolved electronic band structure, we identified these transitions. In the $A_g$ symmetry channel, there is a spectral weight transfer from low-frequency and the formation of a coherence peak around 1200 cm$^{-1}$, which arises from the SDW band-folding-induced intra-orbital transition at the $Z$ point and near the second Dirac point. Moreover, the coherence peak is anisotropic for light polarizations along the AFM and FM directions in detwinned CaFe$_2$As$_2$, directly revealing the inequivalent occupancy of the $d_{xz}$ and $d_{yz}$ orbitals. In the $B_{1g}$ symmetry channel, a Raman scattering peak around 800 cm$^{-1}$ arises from a transition between $d_{xz}$ and $d_{yz}$ at the $\Gamma$ point and reveals the lifted degeneracy of these two orbitals.

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Appendix: Symmetry analysis

In this section we show the details of the orbital symmetry analysis. In Fig. A1, we plot the six dominant Fe 3d orbitals in two different Fe-As layers in a unit cell from the top view at the $\Gamma$, $M$ and $M'$ points. Away from the $\Gamma$ point, the wave function has a phase change of $e^{i\mathbf{k} \cdot \mathbf{R}}$. The parities of these orbitals under all $D_{3h}$ and $D_{2h}$ symmetry operations are listed in Table III and IV.

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FIG. 5. (Color online) \(d_{xy}, d_{yz}\), and \(d_{xz}\) orbitals in two different Fe-As layers in a unit cell in real space at high-symmetry points \(\Gamma, M\) and \(M’\) in the momentum space.
TABLE III. Symmetries of $d_{xy}$, $d_{yz}$, and $d_{xz}$ orbitals at high-symmetry momentum space points in the SDW phase.

| Orbitals | Momentum | $E$ | $C_4(x)$ | $C_2$ | $C_2'''$ | $i$ | $S_4$ | $\sigma_h$ | $\sigma_v$ | $\sigma_d$ | Symmetry |
|----------|----------|-----|----------|-------|---------|-----|-------|----------|----------|----------|-----------|
| $d_{xy}^+$ | $\Gamma$ | 1 | -1 | 1 | 1 | -1 | 1 | -1 | 1 | -1 | $B_{2g}$ |
| $d_{xy}^-$ | $M$ | 2 | 0 | -2 | 0 | 0 | -2 | 0 | 2 | 0 | $E_u$ |
| $d_{xy}^+$ | $M'$ | 2 | 0 | -2 | 0 | 0 | 2 | 0 | -2 | 0 | $E_g$ |
| $d_{xy}^-$ | $\Gamma$ | 1 | 1 | 1 | -1 | -1 | -1 | 1 | -1 | 1 | $A_{2u}$ |
| $d_{xy}^+$ | $M$ | 2 | 0 | -2 | 0 | 0 | 2 | 0 | -2 | 0 | $E_g$ |
| $d_{xy}^-$ | $M'$ | 2 | 0 | -2 | 0 | 0 | 2 | 0 | -2 | 0 | $E_u$ |

Low-temperature paramagnetic phase, $D_{4h}$

| Orbitals | Momentum | $E$ | $C_4(x)$ | $C_2$ | $C_2'''$ | $i$ | $S_4$ | $\sigma_h$ | $\sigma_v$ | $\sigma_d$ | Symmetry |
|----------|----------|-----|----------|-------|---------|-----|-------|----------|----------|----------|-----------|
| $d_{xy}^+$ | $\Gamma$ | 1 | -1 | 1 | 1 | -1 | 1 | -1 | 1 | -1 | $B_{2g}$ |
| $d_{xy}^-$ | $M$ | 2 | 0 | -2 | 0 | 0 | -2 | 0 | 2 | 0 | $E_u$ |
| $d_{xy}^+$ | $M'$ | 2 | 0 | -2 | 0 | 0 | 2 | 0 | -2 | 0 | $E_g$ |
| $d_{xy}^-$ | $\Gamma$ | 1 | 1 | 1 | -1 | -1 | -1 | 1 | -1 | 1 | $A_{2u}$ |
| $d_{xy}^+$ | $M$ | 2 | 0 | -2 | 0 | 0 | 2 | 0 | -2 | 0 | $E_g$ |
| $d_{xy}^-$ | $M'$ | 2 | 0 | -2 | 0 | 0 | 2 | 0 | -2 | 0 | $E_u$ |

TABLE IV. Symmetries of $d_{xy}$, $d_{yz}$, and $d_{xz}$ orbitals at high-symmetry momentum space points in the SDW phase.

| Orbitals | Momentum | $E$ | $C_2(z)$ | $C_2(y)$ | $C_2(x)$ | $i$ | $\sigma_{xy}$ | $\sigma_{xz}$ | $\sigma_{yz}$ | Symmetry |
|----------|----------|-----|----------|----------|----------|-----|---------|----------|----------|-----------|
| $d_{xy}^-$ | $\Gamma$ | 1 | 1 | -1 | -1 | 1 | 1 | -1 | -1 | $B_{1g}$ |
| $d_{xy}^+$ | $M$ | 1 | -1 | 1 | 1 | -1 | 1 | -1 | 1 | $B_{3u}$ |
| $d_{xy}^- | $M'$ | 1 | -1 | 1 | 1 | -1 | 1 | -1 | 1 | $B_{3g}$ |
| $d_{xy}^+ | $\Gamma$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1u}$ |
| $d_{xy}^- | $M$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1g}$ |
| $d_{xy}^+ | $M'$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1g}$ |
| $d_{xy}^- | $\Gamma$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1u}$ |
| $d_{xy}^+ | $M$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1g}$ |
| $d_{xy}^- | $M'$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1u}$ |

Low-temperature SDW phase, $D_{2h}$

| Orbitals | Momentum | $E$ | $C_2(z)$ | $C_2(y)$ | $C_2(x)$ | $i$ | $\sigma_{xy}$ | $\sigma_{xz}$ | $\sigma_{yz}$ | Symmetry |
|----------|----------|-----|----------|----------|----------|-----|---------|----------|----------|-----------|
| $d_{xy}^- | $\Gamma$ | 1 | 1 | -1 | -1 | 1 | 1 | -1 | -1 | $B_{1g}$ |
| $d_{xy}^+ | $M$ | 1 | -1 | 1 | 1 | -1 | 1 | -1 | 1 | $B_{3u}$ |
| $d_{xy}^- | $M'$ | 1 | -1 | 1 | 1 | -1 | 1 | -1 | 1 | $B_{3g}$ |
| $d_{xy}^+ | $\Gamma$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1u}$ |
| $d_{xy}^- | $M$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1g}$ |
| $d_{xy}^- | $M'$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1g}$ |
| $d_{xy}^+ | $\Gamma$ | 1 | -1 | 1 | 1 | -1 | 1 | -1 | 1 | $A_{1u}$ |
| $d_{xy}^- | $M$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1g}$ |
| $d_{xy}^- | $M'$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | $A_{1u}$ |