

## Single crystal raman spectroscopy of cerussite

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### ABSTRACT

Raman and infrared active modes of cerussite were assigned according to their symmetry species and compared to other aragonite group minerals. Small satellite bands at 823 and 1031  $\text{cm}^{-1}$  on the low-wavenumber side of the fundamental vibrations  $\nu_2$  and  $\nu_1$ , respectively, have been assigned to the isotopic substitutions of  $^{13}\text{C}$  and  $^{18}\text{O}$ . The Raman active  $\nu_1$  and  $\nu_2$  carbonate modes are observed at 1051 and 835  $\text{cm}^{-1}$ . The absence of the  $B_{2g}$  component of the  $\nu_1$  and  $\nu_2$  vibrations has been explained by the small coupling between the  $A_g$  and  $B_{2g}$  modes. The Raman active  $\nu_3$  carbonate anti-symmetric stretching mode is observed at 1361 ( $A_g$ ), 1376 ( $B_{1g}$ ), 1419 ( $B_{3g}$ ), and 1477 ( $B_{2g}$ )  $\text{cm}^{-1}$ , while the corresponding infrared active bands are observed at 1396, 1432, and 1456  $\text{cm}^{-1}$ . The Raman active  $\nu_4$  carbonate bending mode is observed at 673 ( $A_g$ ), 668 ( $B_{2g}$ ), 681 ( $B_{1g}$ ), and 694 ( $B_{2g}$ )  $\text{cm}^{-1}$ . The corresponding infrared bands are observed at 670, 679, and 698  $\text{cm}^{-1}$ . In both  $\nu_3$  and  $\nu_4$  the factor group splitting between the  $B_{1g}$  and  $B_{3g}$  modes is 1 to 3 times smaller than the separation of the  $A_g$  and  $B_{2g}$  modes. Raman active lattice vibrations are detected at 120 ( $B_{3g}$ ), 132 ( $A_g$ ), 148 ( $B_{1g}$ ), 152 ( $B_{2g}$ ), 174 ( $B_{2g}$ ), 179 ( $B_{1g}$ ), 213 ( $A_g$ ), 226 ( $B_{3g}$ ), and 243  $\text{cm}^{-1}$  ( $B_{2g}$ ). Corresponding infrared active bands are detected at 573, 543, 573, 423, 375, 290, 205, 165, 146, and 134  $\text{cm}^{-1}$ . Raman bands at 949, 966, 989, 1000, and 1104  $\text{cm}^{-1}$  and at 922, 946, 967, 988, 996, and 1007  $\text{cm}^{-1}$  in the infrared spectra are assigned to combination and overtone bands. Raman bands at 1676 ( $A_g$ ), 1689 ( $A_g$ ), 1730 ( $B_{3g}$ ), and 1740 ( $B_{1g}$ )  $\text{cm}^{-1}$  are ascribed to combination modes of  $\nu_1 + \nu_4$  with bands at 2052 and 2092  $\text{cm}^{-1}$  assigned to  $2\nu_1$ . Corresponding infrared bands are observed at 1729 and 1740  $\text{cm}^{-1}$  ( $\nu_1 + \nu_3$ ). Bands at 2359, 2409, 2471, and 2521  $\text{cm}^{-1}$  are ascribed to  $\nu_1 + \nu_3$ , with broad bands at 1246 and 1323  $\text{cm}^{-1}$  assigned to  $2\nu_4$  modes.