$CO_3$ 

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 $\mathcal{U}_2$ 

99304r Mean vibrational amplitudes, the Bastiansen-Morino shrinkage effect, and thermodynamic functions of some isotopically labeled molecules of carbon trioxide. G. Nagarajan and James R. Durig (Univ. of South Carolina, Columbia, S.C.). Monatsh. Chem. 99(2), 473–83(1968)(Ger). Mean amplitudes of vibration for the bonded as well as nonbonded atom pairs and Bastiansen-Morino shrinkage effect for the isotopic species of carbon trioxide such as  ${}^{12}\text{C}^{16}\text{O}_3$ ,  ${}^{12}\text{C}^{18}\text{O}_3$ , and  ${}^{12}\text{C}^{10}\text{O}_3$  have been computed at T=298 and  $T=500^{\circ}\text{K}$ . by group theoretical method by using symmetry coordinates. Molar thermodynamic functions have also been calcd. for  $200-2000^{\circ}\text{K}$ . on the basis of a

rigid rotator, harmonic oscillator model. Results are briefly

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discussed.

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87: 173175k Thermodynamic isotope effect of trigonal planar and tetrahedral molecules. Kotaka, Masahiro; Kakihana, Hidetaka (Japan). Bull. Res. Lab. Nucl. React. (Tokyo Inst. Technol.) 1977, 2, 13-29 (Eng). The reduced partition function ratios of trigonal planar and tetrahedral mols., CO32-, NO3- SO3, PO3, CF4, CCl4, CBr4, CI4, SO42-, SiO44-, SiF4, SiCl4, SiBr4, SiI4, GeF4, GeCl4, GeBr4, GeI4, MnO4-, and MnO42were calcd. at 200-2000 K from the spectroscopic data. The contribution of each vibrational frequency to these values was also evaluated. At ≥300 K, to a good approxn., the reduced partition function ratios for central atom in a tetrahedral mol. may be calcd. by using only a normal vibrational frequency vs. A linear relationship between the reduced partition function ratios

for central atoms in halides and the stretching force consts.



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