

Mean Amplitudes of Vibration and the Linear Shrinkage Effect in Sulphur Dicyanide

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Pierce *et al.*¹ have recently carried out a normal-coordinate analysis of the vibrations of sulphur dicyanide, making it possible to compute the mean amplitudes of vibration² for this compound. The mentioned workers¹ also demonstrated the linearity of SCN chains to be present, at least to a high degree of accuracy. For this reason the molecule has particular interest because of the linear Bastiansen-Morino shrinkage effect,³ which is accessible from the harmonic-vibrations analysis.

The present computations were based on the bent symmetrical $S(CN)_2$ model with linear SCN chains; symmetry C_{2v} . One used an initial force field with six force constants from Pierce *et al.*¹ These force constants were adjusted to fit accurately the observed vibrational frequencies,¹ whereby more nonvanishing interaction force constants were introduced. It is not the intention to specify here the final force field used in the present calculations. Table 1

Table 1. Mean amplitudes of vibration (u), and linear shrinkage effect (δ) for sulphur dicyanide; Å units.

Quantity		$T = 0$	298°K
$u(S-C)$	(1.701)	0.0439	0.0455
$u(C\equiv N)$	(1.156)	0.0349	0.0349
$u(SN)$	(2.857)	0.0465	0.0484
$u(CC)$	(2.574)	0.0767	0.0987
$u(CN)$	(3.531)	0.0861	0.1260
$u(NN)$	(4.323)	0.1049	0.1810
$\delta(SN)$		0.00776	0.01160

shows the calculated mean amplitudes of vibration. The interatomic distances used as equilibrium values are shown in parentheses for each atom pair. The table also includes the results for the linear Bastiansen-Morino shrinkage effect. The

quantities are given at the temperatures of absolute zero and 298°K.

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Oxidative Conversion of 3-Methoxy-4-hydroxyphenyl (Vanyl)* Compounds to Fluorescent Substances

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Recently, two independent methods for the quantitative determination of homovanillic acid (3-methoxy-4-hydroxyphenylacetic acid or vanylacetic acid, VAA) have been developed, based upon a strong blue fluorescence emitted after oxidation of the acid. In the method of Sharman¹ VAA is oxidized with ferric chloride in an acid medium with subsequent alkalization, whereas Andén, Roos and Werdinius² employ potassium ferricyanide as oxidant in an alkaline medium. The fluorescent compound has been isolated, and its chemical structure established as 2,2'-dihydroxy-3,3'-dimethoxy-biphenyl-5,5'-diacetic acid.³

However, neither of these methods is specific for VAA. A fluorescence of the same nature is exhibited by vanylethylamine (VEA), vanylacetamide, some vanyl- α -alkylacetic acids and their amides,³ as well

* See Gjessing⁹ for a proposed nomenclature of aromatic amino acid metabolites.