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Spectroscopy Letters

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713597299>

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To cite this Article Brendsdal, Egil(1988) 'Symmetry Coordinates of Molecular Vibrations of “Footballene” C_{60} ', Spectroscopy Letters, 21: 4, 319 — 339

To link to this Article: DOI: 10.1080/00387018808082309

URL: <http://dx.doi.org/10.1080/00387018808082309>

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SYMMETRY COORDINATES OF MOLECULAR VIBRATIONS OF
"FOOTBALLENE" C_{60}

Keywords: C_{60} , Footballene, Symmetry coordinates

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ABSTRACT

A complete set of the 174 symmetry coordinates for the C_{60} molecular model referred to as footballene is reported. The model is the truncated icosahedron (symmetry I_h). Hence in addition to triple degeneracy also quadruple and quintuple degeneracies occur.

INTRODUCTION

The already famous experiment by Kroto et al. [1] of laser vaporization of graphite into a helium stream has aroused a great deal of enthusiasm. The experiment was interpreted ("data are compelling" [2]) in terms of cluster formation, where C_{60} dominates the picture, as detected by mass spectra.

In the original publication Kroto et al. [1] proposed a model for the C_{60} compound with the atoms in the vertices of a truncated icosahedron. This model satisfies the tetravalency of carbon in a completely conjugated (sp^2 -hybridized) arrangement.

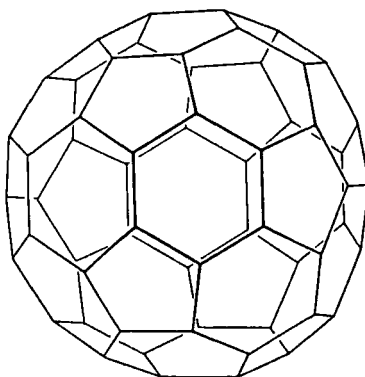


Fig. 1. The model of C_{60}
"footballene".

The (hypothetic) molecule was named "buckminsterfullerene" [1], but for obvious reasons more frequently termed "footballene" in later publications. It has namely the nearly spherical shape of a football (in United States, a soccerball). Twelve pentagons and twenty hexagons are distinguished on its surface. The symmetry group is I_h . The model is shown in Fig. 1.

The C_{60} model of footballene was proposed independently by Haymet [3] and others (see references in [2]). As a conclusion of a considerable amount of theoretical works and discussions, which all appeared in 1986 [4-10], it seems to be a general agreement that footballene would be the most stable C_{60} structure in comparison with several alternatives, and that this structure may account for the "superstability" in consistence with the extremely violent conditions under its formation [1].

The very recent publication [11] from 1987 will probably set an end to this discussion. Thermodynamical data calculated by an MNDO method seem to prove unequivocally that footballene would be the most stable molecule among other C_{60} structures.

On the background of the great interest in footballene it was supposed that an analysis of its molecular vibrations would

be a welcome contribution. At the same time this is a challenging task from the theoretical/mathematical point of view.

Altogether there are relatively few vibrational analyses available for icosahedral models. An analysis of the X_{12} icosahedral-cage model is due to Weber and Thorpe [12], who also performed a normal coordinate analysis for some dodecaborane anions, but did not specify any details on symmetry coordinates. A complete set of symmetry coordinates for the X_{12} model under consideration was published for the first time by Boyle and Parker [13]. The same problem was solved (using a different approach) by Cyvin and Cyvin [14]. Group-theoretical details for the symmetry group I by Fernandez Gomez et al. [15] is also a significant contribution. In a later, excellent work Cyvin et al. [16] succeeded to extend their analysis of the X_{12} symmetry coordinates to the double-icosahedron, $X_{12}Y_{12}$, and reported a normal coordinate analysis for the dodecaborane ion [16] and halogenated dodecaborane ions [17]. No treatment of symmetry coordinates for an icosahedral model with more than 24 atoms has been located in the literature.

In the present work a complete set of independent symmetry coordinates for the molecular vibrations of the 60-atomic footballene model is developed. The coordinates are intended to be used in a normal coordinate analysis in order to calculate the vibrational frequencies of footballene, C_{60} .

VALENCE COORDINATES

Figure 2(a) shows the regular icosahedron with the numbering of its 12 vertices and 30 edges. These edges define the 30 r_i stretching coordinates, which were adapted directly to the truncated icosahedron (footballene).

Three additional types of valence coordinates were defined in footballene, viz. d (stretching), ϕ (bending) and τ ("boat" torsion). Fig 2(b) exemplifies these three types as they emerge around one of the pentagons, incidently No. 3 (encircled numeral).

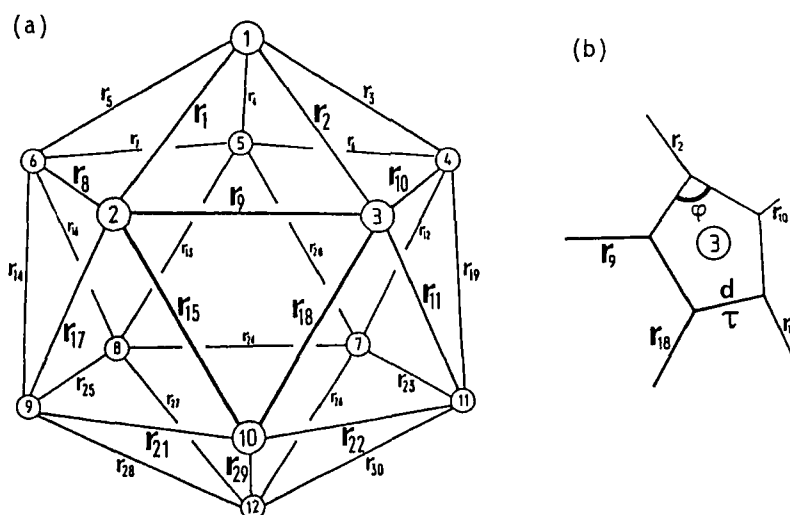


Fig. 2. (a) The regular icosahedron model with numbering of vertices and r_i coordinates. (b) One pentagon in the truncated icosahedron with the d -, ϕ - and τ -type coordinates exemplified. The particular "boat" torsion (τ) involves the bonds r_{11} , $d_{3(1)}$ and r_{18} .

The precise designations of these coordinates are $d_{3(1)}$, $\phi_{3(1)}$ and $\tau_{3(1)}$, where the pentagon number is the first part of the subscript. Figure 3 shows a projection of the footballene model into a plane with numbered pentagons: $j = 1, 2, \dots, 12$ (corresponding to the numbering of vertices in the icosahedron of Fig. 2). All $d_{j(1)}$ stretchings are indicated by double lines. The sense of rotation, as indicated by arrows, serves to define the sets of coordinates $d_{j(2)}$, $d_{j(3)}$, $d_{j(4)}$, $d_{j(5)}$, and likewise for $\phi_{j(i)}$ and $\tau_{j(i)}$; $i = 1, 2, 3, 4, 5$. Notice that the sense of rotation is consistently counterclockwise when the model is viewed from the outside. Figure 4 tends to explain this feature. (It is recommended to inspect a real soccerball, which makes this point immediately lucid.)

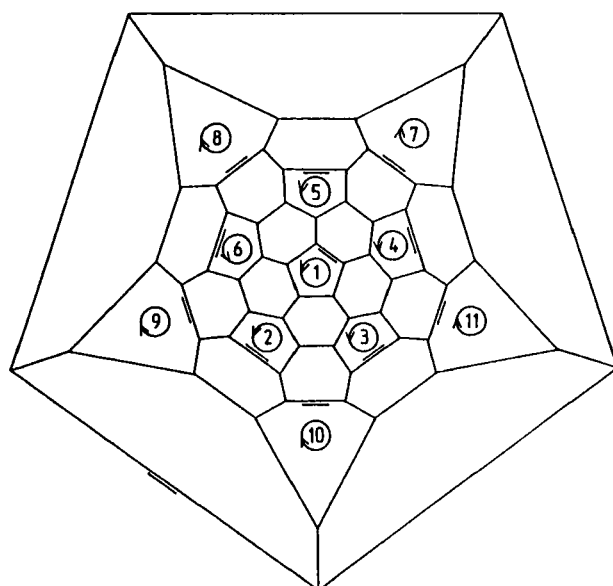


Fig. 3. Projection into a plane of the footballene model. The pentagons are numbered (the outer one being No. 12). See also the text.

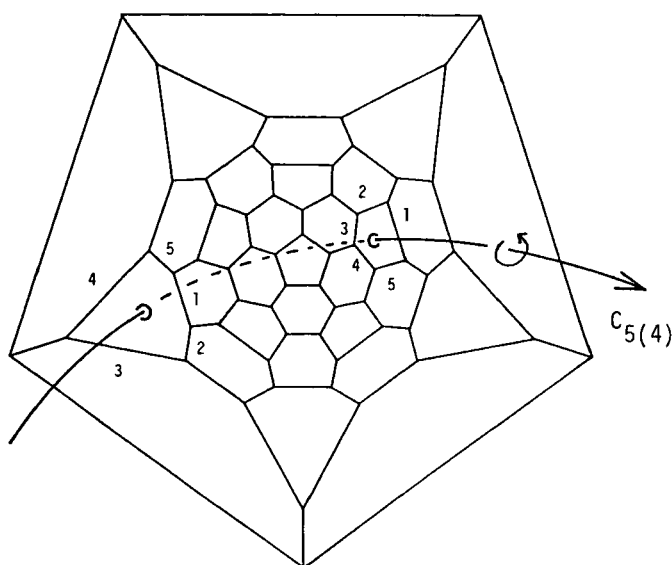


Fig. 4. Explanation of the sense of rotation for the five-fold symmetry axis through the centers of pentagons No. 4 and No. 9.

LINEAR COMBINATIONS OF VALENCE COORDINATES

The $r_1, \dots, r_{30}$ coordinates were grouped into symmetrically equivalent coordinates in relation to the C_5 group with reference to the vertical fivefold symmetry axis. Specifically:

Set No.	Coordinates
1	$r_1, \dots, r_5$
2	$r_6, \dots, r_{10}$
3	$r_{11}, \dots, r_{15}$
4	$r_{16}, \dots, r_{20}$
5	$r_{21}, \dots, r_{25}$
6	$r_{26}, \dots, r_{30}$

The following linear combinations were generated by means of the projection operators of the C_5 group; the superscripts refer to the species of this group.

$$\begin{aligned}
 L_1^A &= r_1 + r_2 + r_3 + r_4 + r_5 \\
 L_1^{E1a} &= r_1 + \alpha r_2 + \beta r_3 + \beta r_4 + \alpha r_5 \\
 L_1^{E1b} &= \gamma r_2 + \delta r_3 - \delta r_4 - \gamma r_5 \\
 L_1^{E2a} &= r_1 + \beta r_2 + \alpha r_3 + \alpha r_4 + \beta r_5 \\
 L_1^{E2b} &= \delta r_2 - \gamma r_3 + \gamma r_4 - \delta r_5
 \end{aligned}$$

The corresponding combinations are formed for the other sets, viz. $L_2^A, L_3^A, \dots, L_6^A, L_2^{E1a}, \dots, L_6^{E2b}$. Here, and throughout this paper, the symbols $\alpha, \beta, \gamma, \delta$ are used to designate the following constants.

$$\begin{aligned}
 \alpha &= \cos \frac{2\pi}{5} = \frac{1}{4}(\sqrt{5} - 1), & \gamma &= \sin \frac{2\pi}{5} = \frac{1}{4}\sqrt{10 + 2\sqrt{5}} \\
 \beta &= \cos \frac{4\pi}{5} = -\frac{1}{4}(\sqrt{5} + 1), & \delta &= \sin \frac{4\pi}{5} = \frac{1}{4}\sqrt{10 - 2\sqrt{5}}
 \end{aligned}$$

The linear combinations for the d-, ϕ - and τ -type coordinates are more complicated, although they follow the same scheme as above. We define:

$$\begin{aligned}
 K_1^A(d) &= d_{1(1)} + d_{1(2)} + d_{1(3)} + d_{1(4)} + d_{1(5)} \\
 K_1^{E1a}(d) &= d_{1(1)} + \alpha d_{1(2)} + \beta d_{1(3)} + \beta d_{1(4)} + \alpha d_{1(5)}
 \end{aligned}$$

$$K_1^{E1b}(d) = \gamma d_{1(2)} + \delta d_{1(3)} - \delta d_{1(4)} - \gamma d_{1(5)}$$

$$K_1^{E2a}(d) = d_{1(1)} + \beta d_{1(2)} + \alpha d_{1(3)} + \alpha d_{1(4)} + \beta d_{1(5)}$$

$$K_1^{E2b}(d) = \delta d_{1(2)} - \gamma d_{1(3)} + \gamma d_{1(4)} - \delta d_{1(5)}$$

The corresponding combinations are now formed for K_2^A , K_3^A , ..., K_{12}^A , K_2^{E1a} , ..., K_{12}^{E2b} . Furthermore, the d coordinates may be replaced by ϕ 's or τ 's throughout.

SYMMETRICAL STRUCTURE

The symmetry coordinates are distributed into the species of the I_h group in the following way.

$$\begin{aligned} \Gamma_{\text{vib}} = & 2A_g(A) + 3T_{1g}(A+E_1) + 4T_{2g}(A+E_2) + 6G_g(E_1+E_2) + 8H_g(A+E_1+E_2) \\ & + A_u(A) + 4T_{1u}(A+E_1) + 5T_{2u}(A+E_2) + 6G_u(E_1+E_2) + 7H_u(A+E_1+E_2) \end{aligned}$$

The correlations with the species of the C_5 group are included in parentheses.

SYMMETRY COORDINATES

A complete set of independent symmetry coordinates was produced by applying the projection operator techniques to the linear combinations of valence coordinates (see above) with reference to the species of the I_h group. The result is specified in the following.

Normalization factors are not given in the above listing. They were determined numerically by a computer program, into which the symmetry coordinates were coded. A series of programs available at the present laboratory were actually used during the development of the coordinates and for checking their correctness. In the first place they were checked for orthogonality. Next the G matrix was computed (as a 174×174 matrix) in order to assure that (a) all interaction terms between symmetry coordinates of different species vanish, and (b) all degenerate sets of coordinates give identical and non-coupling G matrix blocks. This

$$\begin{aligned}
S_{Ag1}(\tau) &= L_1^A + L_2^A + L_3^A + L_4^A + L_5^A + L_6^A \\
S_{Ag2}(d) &= K_1^A + K_2^A + K_3^A + K_4^A + K_5^A + K_6^A \\
S_{T1g\bar{a}1}(d) &= K_7^A + K_8^A + K_9^A + K_{10}^A + K_{11}^A + K_{12}^A \\
S_{T1g\bar{a}2}(\tau) &= K_7^{F1b} + K_8^{F1b} + K_9^{F1b} + K_{10}^{F1b} + K_{11}^{F1b} + K_{12}^{F1b} \\
S_{T1g\bar{a}2}(\tau) &= K_7^{F1a} + K_8^{F1a} + K_9^{F1a} + K_{10}^{F1a} + K_{11}^{F1a} + K_{12}^{F1a} \\
S_{T1g\bar{a}3}(\tau) &= \sqrt{5} K_1^A + K_2^A + K_3^A + K_4^A + K_5^A + K_6^A \\
S_{T1g\bar{b}1}(d) &= K_1^{F1a} + K_2^{F1a} + K_3^{F1a} + K_4^{F1a} + K_5^{F1a} + K_6^{F1a} \\
S_{T1g\bar{b}2}(\tau) &= K_7^{F1b} + K_8^{F1b} + K_9^{F1b} + K_{10}^{F1b} + K_{11}^{F1b} + K_{12}^{F1b} \\
S_{T1g\bar{b}3}(\tau) &= K_7^{F1b} + K_8^{F1b} + K_9^{F1b} + K_{10}^{F1b} + K_{11}^{F1b} + K_{12}^{F1b} \\
S_{T1g\bar{a}1}(d) &= K_7^{F1b} + K_8^{F1b} + K_9^{F1b} + K_{10}^{F1b} + K_{11}^{F1b} + K_{12}^{F1b} \\
S_{T1g\bar{a}2}(\tau) &= K_7^{F1a} + K_8^{F1a} + K_9^{F1a} + K_{10}^{F1a} + K_{11}^{F1a} + K_{12}^{F1a} \\
S_{T1g\bar{a}3}(\tau) &= K_7^{F1a} + K_8^{F1a} + K_9^{F1a} + K_{10}^{F1a} + K_{11}^{F1a} + K_{12}^{F1a} \\
S_{T2g\bar{a}1}(d) &= K_7^{F2b} + K_8^{F2b} + K_9^{F2b} + K_{10}^{F2b} + K_{11}^{F2b} + K_{12}^{F2b} \\
S_{T2g\bar{a}2}(\vartheta) &= K_7^{F2b} + K_8^{F2b} + K_9^{F2b} + K_{10}^{F2b} + K_{11}^{F2b} + K_{12}^{F2b}
\end{aligned}$$

[illegible]

$$\begin{aligned}
S_{\mathcal{O}g\overline{2}6}(1) &= -\kappa_2^{F2b} + \gamma \frac{\kappa_3^{F2a}}{\kappa_3} - \alpha \kappa_3^3 + \frac{\delta \kappa_4^{F2a}}{\delta} \kappa_3^3 - \beta \kappa_4^4 - \gamma \frac{\kappa_5^{F2a}}{\kappa_5} - \alpha \kappa_5^5 - \gamma \frac{\kappa_6^{F2a}}{\kappa_6} - \beta \kappa_6^6 \\
&+ \kappa_7^{F2b} - \gamma \frac{\kappa_8^{F2a}}{\kappa_8} + \alpha \kappa_8^8 - \frac{\delta \kappa_9^{F2a}}{\delta} \kappa_8^8 + \beta \kappa_9^9 + \kappa_{10}^{F2b} + \kappa_{11}^{F2b} + \kappa_{12}^{F2b} + \alpha \kappa_{13}^{F2b} + \beta \kappa_{14}^{F2b} + \gamma \frac{\kappa_{15}^{F2a}}{\kappa_{15}} - \delta \kappa_{16}^{F2b} \\
&+ \kappa_{17}^{F2b} + \alpha \kappa_{18}^{F2b} + \beta \kappa_{19}^{F2b} + \gamma \frac{\kappa_{20}^{F2a}}{\kappa_{20}} - \delta \kappa_{21}^{F2b} + \alpha \kappa_{22}^{F2b} + \beta \kappa_{23}^{F2b} + \gamma \frac{\kappa_{24}^{F2a}}{\kappa_{24}} - \delta \kappa_{25}^{F2b} + \alpha \kappa_{26}^{F2b} + \beta \kappa_{27}^{F2b} + \gamma \frac{\kappa_{28}^{F2a}}{\kappa_{28}} - \delta \kappa_{29}^{F2b} + \alpha \kappa_{30}^{F2b} + \beta \kappa_{31}^{F2b} + \gamma \frac{\kappa_{32}^{F2a}}{\kappa_{32}} - \delta \kappa_{33}^{F2b} + \alpha \kappa_{34}^{F2b} + \beta \kappa_{35}^{F2b} + \gamma \frac{\kappa_{36}^{F2a}}{\kappa_{36}} - \delta \kappa_{37}^{F2b} + \alpha \kappa_{38}^{F2b} + \beta \kappa_{39}^{F2b} + \gamma \frac{\kappa_{40}^{F2a}}{\kappa_{40}} - \delta \kappa_{41}^{F2b} + \alpha \kappa_{42}^{F2b} + \beta \kappa_{43}^{F2b} + \gamma \frac{\kappa_{44}^{F2a}}{\kappa_{44}} - \delta \kappa_{45}^{F2b} + \alpha \kappa_{46}^{F2b} + \beta \kappa_{47}^{F2b} + \gamma \frac{\kappa_{48}^{F2a}}{\kappa_{48}} - \delta \kappa_{49}^{F2b} + \alpha \kappa_{50}^{F2b} + \beta \kappa_{51}^{F2b} + \gamma \frac{\kappa_{52}^{F2a}}{\kappa_{52}} - \delta \kappa_{53}^{F2b} + \alpha \kappa_{54}^{F2b} + \beta \kappa_{55}^{F2b} + \gamma \frac{\kappa_{56}^{F2a}}{\kappa_{56}} - \delta \kappa_{57}^{F2b} + \alpha \kappa_{58}^{F2b} + \beta \kappa_{59}^{F2b} + \gamma \frac{\kappa_{60}^{F2a}}{\kappa_{60}} - \delta \kappa_{61}^{F2b} + \alpha \kappa_{62}^{F2b} + \beta \kappa_{63}^{F2b} + \gamma \frac{\kappa_{64}^{F2a}}{\kappa_{64}} - \delta \kappa_{65}^{F2b} + \alpha \kappa_{66}^{F2b} + \beta \kappa_{67}^{F2b} + \gamma \frac{\kappa_{68}^{F2a}}{\kappa_{68}} - \delta \kappa_{69}^{F2b} + \alpha \kappa_{70}^{F2b} + \beta \kappa_{71}^{F2b} + \gamma \frac{\kappa_{72}^{F2a}}{\kappa_{72}} - \delta \kappa_{73}^{F2b} + \alpha \kappa_{74}^{F2b} + \beta \kappa_{75}^{F2b} + \gamma \frac{\kappa_{76}^{F2a}}{\kappa_{76}} - \delta \kappa_{77}^{F2b} + \alpha \kappa_{78}^{F2b} + \beta \kappa_{79}^{F2b} + \gamma \frac{\kappa_{80}^{F2a}}{\kappa_{80}} - \delta \kappa_{81}^{F2b} + \alpha \kappa_{82}^{F2b} + \beta \kappa_{83}^{F2b} + \gamma \frac{\kappa_{84}^{F2a}}{\kappa_{84}} - \delta \kappa_{85}^{F2b} + \alpha \kappa_{86}^{F2b} + \beta \kappa_{87}^{F2b} + \gamma \frac{\kappa_{88}^{F2a}}{\kappa_{88}} - \delta \kappa_{89}^{F2b} + \alpha \kappa_{90}^{F2b} + \beta \kappa_{91}^{F2b} + \gamma \frac{\kappa_{92}^{F2a}}{\kappa_{92}} - \delta \kappa_{93}^{F2b} + \alpha \kappa_{94}^{F2b} + \beta \kappa_{95}^{F2b} + \gamma \frac{\kappa_{96}^{F2a}}{\kappa_{96}} - \delta \kappa_{97}^{F2b} + \alpha \kappa_{98}^{F2b} + \beta \kappa_{99}^{F2b} + \gamma \frac{\kappa_{100}^{F2a}}{\kappa_{100}} - \delta \kappa_{101}^{F2b} + \alpha \kappa_{102}^{F2b} + \beta \kappa_{103}^{F2b} + \gamma \frac{\kappa_{104}^{F2a}}{\kappa_{104}} - \delta \kappa_{105}^{F2b} + \alpha \kappa_{106}^{F2b} + \beta \kappa_{107}^{F2b} + \gamma \frac{\kappa_{108}^{F2a}}{\kappa_{108}} - \delta \kappa_{109}^{F2b} + \alpha \kappa_{110}^{F2b} + \beta \kappa_{111}^{F2b} + \gamma \frac{\kappa_{112}^{F2a}}{\kappa_{112}} - 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\delta \kappa_{209}^{F2b} + \alpha \kappa_{210}^{F2b} + \beta \kappa_{211}^{F2b} + \gamma \frac{\kappa_{212}^{F2a}}{\kappa_{212}} - \delta \kappa_{213}^{F2b} + \alpha \kappa_{214}^{F2b} + \beta \kappa_{215}^{F2b} + \gamma \frac{\kappa_{216}^{F2a}}{\kappa_{216}} - \delta \kappa_{217}^{F2b} + \alpha \kappa_{218}^{F2b} + \beta \kappa_{219}^{F2b} + \gamma \frac{\kappa_{220}^{F2a}}{\kappa_{220}} - \delta \kappa_{221}^{F2b} + \alpha \kappa_{222}^{F2b} + \beta \kappa_{223}^{F2b} + \gamma \frac{\kappa_{22$$

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test involves the triple, quadruple and quintuple degeneracies. Finally the G matrix was inverted in order to assure that it is not singular.

Acknowledgements: The author thanks Professor S.J. Cyvin, who suggested the problem, for helpful discussions, and Sivilingeniør B.N. Cyvin with Førsteamanuensis J. Brunvoll for instructions in using the computer programs.

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Date Received: 12/02/87
Date Accepted: 01/18/88