The Crystal Structure of Tellurium(IV) Catecholate, 
\[ \text{Te(C}_6\text{H}_4\text{O}_2)_2 \]

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The positions of the oxygen and carbon atoms in the structure of tellurium(IV) catecholate, \( \text{Te(C}_6\text{H}_4\text{O}_2)_2 \), have been determined. Tellurium(IV) catecholate forms monoclinic crystals with the cell dimensions \( a = 22.678 \) Å, \( b = 6.9354 \) Å, \( c = 16.5274 \) Å, and \( \beta = 123.15^\circ \), belonging to the space group \( C2/c \).

The structure was solved by means of three-dimensional electron density calculations and refined by least squares methods, using 780 independent reflexions, a final \( R \) value of 0.105 being obtained.

Tellurium is four-fold co-ordinated by oxygen, all four oxygen atoms lying on the same side of the tellurium atom. The four Te—O bond distances range from 1.97 Å to 2.11 Å, the standard deviations being 0.02 Å. There is, in addition, a further oxygen atom situated at a distance of 2.64 Å from the tellurium atom on the side opposite to the four Te—O bonds. Since this latter oxygen atom belongs to another \( \text{Te(C}_6\text{H}_4\text{O}_2)_2 \) unit, a chainlike structure results.

The crystal structure of tellurium(IV) catecholate, \( \text{Te(C}_6\text{H}_4\text{O}_2)_2 \), has been determined in connection with a series of investigations of tellurium compounds containing tellurium-oxygen bonds.

Tellurium(IV) catecholate was studied in 1959 by Antikainen and Lundgren.\(^1\) The space group was found to be \( C2/c \), and the tellurium atoms were assigned the general position \( 8(f) \) with \( x = 0.236, y = 0.165, \) and \( z = 0.175 \), by interpreting the Patterson projections \( P(uwp) \) and \( P(uwp) \), and the generalized Patterson function \( P_1(uwp) \). These results were taken to be the starting point of the present investigation.

**EXPERIMENTAL**

Crystals of tellurium(IV) catecholate were prepared according to Antikainen and Mäkäräinen.\(^2\) Yellow needles were obtained, the majority of which were twinned, but it was possible to pick out a few single crystals suitable for X-ray work with Weissenberg methods. The crystal used in the investigation was a needle of length 0.3 mm (\( b \) axis direction) and cross-section 0.03 × 0.025 mm. The \( b \) axis was chosen as rotation axis,
Table I. Guinier powder photograph of Te(C₄H₄O₂)ₓ, CuKα₁ radiation. \( \lambda (\text{CuKα₁}) = 1.54050 \text{Å} \).

| \( h \) | \( k \) | \( l \) | \( 10^4 \sin^2 q \) | \( 10^4 \sin^2 q \) | \( |F| \times 10^{-1} \) | \( I \) |
|-----|-----|-----|----------|----------|----------------|-----|
| 20  | 0   | 0   | 659      | 668      | 52             | vvs |
| 20  | -2  |     | 911      | 910      | 34             | vs  |
| 00  | 2   |     | 1243     | 1240     | 16             | w   |
| 11  | 0   |     | 1399     | 1398     | 21             | vvw |
| 11  | -1  |     | 1458     | 1461     | 25             | s   |
| 40  | -2  |     | 1896     | 1897     | 27             | m   |
| 11  | 1   |     | 1953     | 1955     | 21             | m   |
| 11  | -2  |     | 2137     | 2144     | 20             | s   |
| 31  | -2  |     | 2466     | 2472     | 8              | vvw |
| 40  | 0   |     | 2629     | 2633     | 25             | w   |
| 11  | 2   |     | 3125     | 3132     | 25             | s   |
| 31  | -3  |     | 3279     | 3281     | 28             | s   |
| 11  | -3  |     | 3444     | 3447     | 23             | s   |
| 40  | -4  |     | 3653     | 3640     | 7              | vvw |
| 20  | -4  |     | 3633     | 3641     | 14             | m   |
| 31  | 1   |     | 3782     | 3766     | 24             | m   |
| 60  | -2  |     | 4199     | 4200     | 54             | m   |
| 51  | -3  |     | 4428     | 4432     | 27             | w   |
| 02  | 0   |     | 4833     | 4834     | 22             | s   |
| 11  | 3   |     | 4933     | 4929     | 32             | w   |
| 00  | 4   |     | 4952     | 4959     | 30             | w   |
| 02  | 1   |     | 5235     | 5244     | 20             | w   |
| 51  | -4  |     | 5361     | 5366     | 18             | s   |
| 11  | -4  |     | 5361     | 5369     | 27             | s   |
| 22  | -1  |     | 5398     | 5408     | 22             | w   |
| 22  | 0   |     | 5583     | 5592     | 13             | vvw |
| 02  | 2   |     | 6169     | 6174     | 9              | vvw |
| 22  | -2  |     | 5842     | 5844     | 14             | vvw |
| 22  | 1   |     | 6397     | 6396     | 14             | vvw |
| 31  | -5  |     | 6753     | 6758     | 15             | vvw |
| 42  | -1  |     | 6896     | 6889     | 22             | w   |
| 51  | 1   |     | 6896     | 6893     | 16             | s   |
| 71  | -3  |     | 6896     | 6899     | 28             | w   |
| 71  | -4  |     | 7356     | 7340     | 14             | w   |
| 11  | 4   |     | 7346     | 7345     | 13             | vvw |
| 80  | -4  |     | 7533     | 7587     | 16             | vvw |
| 31  | 3   |     | 7720     | 7727     | 21             | w   |
| 80  | -2  |     | 7817     | 7829     | 42             | w   |
| 11  | -5  |     | 7998     | 7911     | 23             | w   |
| 60  | -6  |     | 8184     | 8189     | 19             | vvw |
| 71  | -5  |     | 8398     | 8400     | 18             | vvw |
| 42  | -4  |     | 8572     | 8574     | 9              | vvw |
| 22  | -4  |     | 8572     | 8575     | 7              | vvw |
| 20  | -6  |     | 8847     | 8852     | 33             | m   |
| 51  | -6  |     | 9101     | 9085     | 12             | vvw |
| 31  | -6  |     | 9421     | 9426     | 17             | w   |
| 62  | -1  |     | 9682     | 9686     | 27             | m   |
| 71  | -6  |     | 10085    | 10080    | 12             | vvw |
| 11  | 5   |     | 10374    | 10382    | 17             | vvw |
| 00  | 6   |     | 11169    | 11159    | 40             | m   |
| 71  | 1   |     | 11343    | 11337    | 15             | vvw |
| 51  | 3   |     | 11844    | 11843    | 20             | vvw |
| 62  | 1   |     | 12661    | 12651    | 14             | vvw |

and Weissenberg photographs of the layers 40l—44l were registered. Multiple film
techniques employing six films for each layer line were used, giving a ratio between the
strongest and the weakest measurable intensities of approximately 2200:1.

In order to determine accurate cell dimensions a Guinier powder photograph was
taken, using KCl as internal standard (CuKα, radiation, \( \lambda = 1.54050 \) Å, \( a_{KCl} = 6.2919 \)
Å at 20°C). 88 lines on the photograph were indexed with the aid of the Algol pro-
gramme POWDER.4 and a list of observed and calculated sin\( ^{\circ} \) values are shown in
Table 1. Using the same programme, a least squares refinement based on these lines
gave the following cell dimensions:

\[
\begin{align*}
a &= 22.678 \pm 0.003 \text{ Å} \\
b &= 6.9355 \pm 0.0008 \text{ Å} \\
c &= 16.5274 \pm 0.0015 \text{ Å} \\
\beta &= 123.154^\circ \pm 0.005^\circ \\
V &= 2176 \text{ Å}^3.
\end{align*}
\]

**DATA PROCESSING**

The intensities were estimated visually using an intensity scale prepared
by making timed exposures of a chosen reflexion of the actual crystal. The

reflexions of the different film layers were scaled together manually, applying a simple weighting scheme based on the reliability of the estimations within different intervals of degrees of blackness of the intensity scale.

Errors in the intensity material due to absorption effects could not be neglected since the calculated value of the linear absorption coefficient for \( \text{Te(C}_6\text{H}_4\text{O}_3)_2 \) was 232 cm\(^{-1}\).\(^5\) The absorption correction was performed using a programme written by Abrahamsson\(^6\) for the SAAB D21 computer.

Lorenz’ and polarization factors were calculated on the same computer with the programme DR written by Abrahamsson and Larsson.\(^6\)

The \( F_c \) values were brought on to an absolute scale by comparison with \( F_c \) only after an approximate structure had been devised.

POSITIONS OF THE LIGHT ATOMS

To obtain maximal resolution in the electron density calculations, the structural parameters of tellurium were refined using the least squares, block diagonal approximation programme written by Wengelin\(^7\) for the SAAB D21 computer. The refinement was based on all 780 observed reflexions, and after five cycles, the \( R \) value dropped to 0.25, and the following parameters were obtained for the tellurium atoms: 8 Te in \( C2/c:8(f) \) with \( x = 0.238, y = 0.168, z = 0.176, \) and \( B = 4.3 \text{ Å}^2 \).

A three-dimensional difference Fourier synthesis, based on the signs obtained from the tellurium parameters, was calculated using the Fourier programme written by Larsson.\(^6\) The positions of all oxygen and carbon atoms in the structure were then apparent, the oxygen atoms occupying four of the general positions \( C2/c:8(f) \) and the carbon atoms twelve positions \( C2/c:8(f) \).

An electron density projection of the structure on the \( xz \) plane is shown in Fig. 1.

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Fig. 1. Electron density projection \( g(xyz) \) of \( \text{Te(C}_6\text{H}_4\text{O}_3)_2 \). The distance between two thin contours or between one thin and one thick contour within the maxima corresponds to 1/10 of that between two thick contours. The final positions of Te (▲), O (■), and C (●) are indicated.

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REFINEMENT OF THE STRUCTURE

The atomic co-ordinates, isotropic temperature factors, and separate scale factors for each layer line were refined, using the least squares, full matrix programme LALS, modified for the CD 3600 computer in Uppsala. Atomic scattering values given by Cromer and Waber were used, and each structure factor was weighted according to the weighting function devised by Cruickshank \( w = (a + F^2 + cF^2 + dF^2)^{-1} \) with \( a = 30 \), \( c = 0.004 \), and \( d = 0 \).

Table 2. Atomic co-ordinates, expressed as fractions of the cell edges, and isotropic thermal parameters in \( \AA^2 \) for Te(C₆H₆O₃)₄.

<table>
<thead>
<tr>
<th>Atom</th>
<th>x</th>
<th>y</th>
<th>z</th>
<th>B</th>
</tr>
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<tbody>
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<tr>
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After four cycles of refinement all parameter shifts became smaller than 5% of the standard deviations and the R value converged to 0.105. The positional co-ordinates and the isotropic temperature factors are given, together with their standard deviations, in Table 2. A comparison between the observed and calculated structure factors is shown in Table 3.

The results of the refinement were supported by the appearance of a three-dimensional \( F_0 \) - \( F_c \) Fourier synthesis, in which no peak denser than 3.3 electrons/\( \AA^3 \) could be detected, the \( F_c \) values being obtained from the parameters of Table 2. The highest peaks in the difference maps occurred in the neighbourhood of the tellurium atoms, and were probably due to diffraction effects not accounted for.

Peaks corresponding to some of the hydrogen atoms attached to the benzene rings could be identified in the final difference Fourier maps. These were not, however, included in the refinement, since it was considered, that the contribution to the structure factors due to the hydrogen atoms could give no significant results in a structure containing such a heavy atom as tellurium, and since only reflexions from one axis were used in the calculations.

Table 3. Calculated and observed structure factors for Te(C₈H₆O₃)₂ (The columns are l, $F_o$, and $F_c$, respectively).

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### Table 3. Continued.

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### SOME GEOMETRICAL CALCULATIONS

The positions of the hydrogen atoms, as calculated by the programme HYDROGENS, assuming \( sp^2 \) hybridization of the carbon atoms and \( C-H \) bond distances of 1.09 \( \AA \) in the benzene rings, are given in Table 4.

The best least squares planes through the carbon atoms of the two benzene rings were calculated using the programme PLANEFIT.\(^7\) The deviations of certain atoms from these planes are shown in Table 5.

### Table 4. Geometrically calculated positions of the hydrogen atoms in \( \text{Te(C}_6\text{H}_4\text{O}_4)\).\(^1\)

<table>
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<th></th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
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<tbody>
<tr>
<td>H(_2)</td>
<td>0.384</td>
<td>0.341</td>
<td>0.158</td>
</tr>
<tr>
<td>H(_4)</td>
<td>0.413</td>
<td>0.034</td>
<td>0.241</td>
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<tr>
<td>H(_6)</td>
<td>0.129</td>
<td>0.220</td>
<td>0.347</td>
</tr>
<tr>
<td>H(_8)</td>
<td>0.201</td>
<td>0.224</td>
<td>0.628</td>
</tr>
<tr>
<td>H(_{10})</td>
<td>0.030</td>
<td>0.274</td>
<td>0.157</td>
</tr>
<tr>
<td>H(_{12})</td>
<td>0.445</td>
<td>0.489</td>
<td>0.099</td>
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<tr>
<td>H(_{14})</td>
<td>0.520</td>
<td>0.174</td>
<td>0.415</td>
</tr>
<tr>
<td>H(_{11})</td>
<td>0.401</td>
<td>0.112</td>
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### Table 5. Best least squares planes through the carbon rings (referred to Cartesian co-ordinates in Ångström) and deviations from these planes.

Transformation to Cartesian co-ordinates \((X,Y,Z):\)

\[
X = 22.678x \\
Y = 6.9356y \\
Z = -9.045z + 13.848z
\]

1. Plane through \( C_1 - C_4: \)

\[-0.9976X + 0.0631Y - 0.0268Z = -3.9000 \, \AA\]

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<th>deviation (Å)</th>
<th>atom</th>
<th>deviation (Å)</th>
</tr>
</thead>
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<td>C(_8)</td>
<td>0.016</td>
</tr>
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<td>-0.015</td>
<td>O(_1)</td>
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</tr>
<tr>
<td>C(_3)</td>
<td>0.017</td>
<td>O(_2)</td>
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<tr>
<td>C(_5)</td>
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</tbody>
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2. Plane through $C_7-C_{12}$:

$$0.1951X + 0.1882Y - 0.9626Z = -1.7558 \text{ Å}$$

<table>
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<tr>
<th>atom</th>
<th>deviation (Å)</th>
<th>atom</th>
<th>deviation (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_7$</td>
<td>0.018</td>
<td>$C_{12}$</td>
<td>-0.033</td>
</tr>
<tr>
<td>$C_8$</td>
<td>0.001</td>
<td>$O_4$</td>
<td>0.032</td>
</tr>
<tr>
<td>$C_9$</td>
<td>-0.005</td>
<td>$O_5$</td>
<td>-0.048</td>
</tr>
<tr>
<td>$C_{10}$</td>
<td>-0.009</td>
<td>$Te$</td>
<td>0.370</td>
</tr>
<tr>
<td>$C_{11}$</td>
<td>0.028</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Angle between the planes: 99.03°

*Table 6.* Distances and angles in the tellurium-oxygen co-ordination polyhedron. (Standard deviations in parentheses).

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>Te—O_1</td>
<td>2.008(28) Å</td>
<td>O_1—O_3</td>
<td>3.442(34) Å</td>
</tr>
<tr>
<td>Te—O_2</td>
<td>1.981(19)</td>
<td>O_1—O_4</td>
<td>3.342(36)</td>
</tr>
<tr>
<td>Te—O_3</td>
<td>1.977(22)</td>
<td>O_2—O_3</td>
<td>2.900(28)</td>
</tr>
<tr>
<td>Te—O_4</td>
<td>2.110(23)</td>
<td>O_2—O_4</td>
<td>2.630(30)</td>
</tr>
<tr>
<td>Te—O_4'</td>
<td>2.644(21)</td>
<td>Te—Te</td>
<td>4.110(02) (2×)</td>
</tr>
</tbody>
</table>

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<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>O_1—Te—O_2</td>
<td>80.9(1.0)°</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O_1—Te—O_3</td>
<td>84.6(0.9)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O_1—Te—O_4</td>
<td>154.3(0.9)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O_2—Te—O_3</td>
<td>98.1(0.8)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O_2—Te—O_4</td>
<td>79.9(0.9)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O_3—Te—O_4</td>
<td>81.4(0.9)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Table 7.* Distances and angles in the catecholate groups. (Standard deviations in parentheses).

<p>| | | | |</p>
<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>O_1—O_2</td>
<td>2.588(36) Å</td>
<td>C_7—C_8—O_1</td>
<td>113.6(3.0)°</td>
</tr>
<tr>
<td>O_1—C_7</td>
<td>1.346(35)</td>
<td>C_7—C_8—O_1</td>
<td>126.6(3.2)</td>
</tr>
<tr>
<td>O_2—C_7</td>
<td>1.400(41)</td>
<td>C_7—C_8—O_2</td>
<td>116.9(2.2)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.423(49)</td>
<td>C_7—C_8—O_3</td>
<td>122.4(3.3)</td>
</tr>
<tr>
<td>C_7—C_8'</td>
<td>1.363(40)</td>
<td>C_7—C_8—C_9</td>
<td>121.0(3.4)</td>
</tr>
<tr>
<td>C_7—C_8'</td>
<td>1.364(61)</td>
<td>C_7—C_8—C_9'</td>
<td>118.5(3.7)</td>
</tr>
<tr>
<td>C_7—C_8'</td>
<td>1.428(65)</td>
<td>C_7—C_8—C_9</td>
<td>122.6(3.3)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.353(52)</td>
<td>C_7—C_8—C_9</td>
<td>118.4(4.1)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.383(55)</td>
<td>C_7—C_8—C_9</td>
<td>119.5(3.9)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.280(26)</td>
<td>C_7—C_8—C_9</td>
<td>120.0(2.6)</td>
</tr>
</tbody>
</table>

<p>| | | | |</p>
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<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>O_2—O_4</td>
<td>2.666(32) Å</td>
<td>C_{12}—C_7—O_4</td>
<td>117.1(2.7)°</td>
</tr>
<tr>
<td>O_2—C_7</td>
<td>1.357(42)</td>
<td>C_7—C_8—O_2</td>
<td>119.5(3.3)</td>
</tr>
<tr>
<td>O_2—C_12</td>
<td>1.392(34)</td>
<td>C_7—C_8—O_3</td>
<td>117.9(2.8)</td>
</tr>
<tr>
<td>O_2—C_12</td>
<td>1.396(51)</td>
<td>C_7—C_8—O_3'</td>
<td>120.8(3.0)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.397(45)</td>
<td>C_7—C_8—C_9</td>
<td>123.3(3.3)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.436(58)</td>
<td>C_7—C_8—C_9</td>
<td>114.7(3.5)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.331(62)</td>
<td>C_7—C_8—C_9</td>
<td>122.7(3.3)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.453(47)</td>
<td>C_7—C_8—C_9</td>
<td>122.4(3.5)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.395(48)</td>
<td>C_7—C_8—C_9</td>
<td>115.3(3.2)</td>
</tr>
<tr>
<td>C_7—C_8</td>
<td>1.395(48)</td>
<td>C_7—C_8—C_9</td>
<td>121.2(2.8)</td>
</tr>
</tbody>
</table>

Interatomic distances and angles together with their standard deviations were calculated with the programme DISTAN \(^8\) and are listed in Tables 6 and 7.

DISCUSSION OF THE STRUCTURE

The basic unit of the structure is formed by the co-ordination of the four oxygen atoms of two catecholate groups to one tellurium atom. Apart from van der Waals' forces between the different formula units, the structure may be considered to be held together by a weak intermolecular bond, corresponding to a Te—O distance of 2.644 Å. From this point of view, the structure may be regarded as being composed of rows of \( \cdots \text{O—TeO}_3\cdots \text{O—TeO}_3\cdots \text{O—TeO}_3\cdots \) running through the structure in the direction of the \( b \) axis, these rows being embedded and isolated from each other by the carbon rings of the catecholate groups.

![Diagram](image)

*Fig. 2. The formula unit of tellurium(IV) catecholate projected on the (101) plane. (The dotted line shows the intermolecular Te—O\(_4\) interaction).*

*A projection of the formula unit on the (101) plane is shown in Fig. 2. In Fig. 3, which shows part of the structure, the short intermolecular Te—O distances are indicated as dotted lines between a few of the molecules in the chain.*

*Fig. 3. Part of the structure of Te(C\(_4\)H\(_4\)O\(_8\))\(_2\).*

*Table 8. Comparison of the tellurium-oxygen co-ordination polyhedra in some Te(IV) compounds. (Standard deviations in the distances and angles are approximately 0.02 Å and 0.9°, respectively).*

<table>
<thead>
<tr>
<th></th>
<th>( \alpha )-TeO(_3)</th>
<th>( \beta )-TeO(_3)</th>
<th>TeO(_3)HNO(_3)</th>
<th>Te(C(_4)H(_4)O(_8))(_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Te—O (axial)</td>
<td>2.07 Å (2x)</td>
<td>2.07 Å</td>
<td>2.02 Å</td>
<td>2.01 Å</td>
</tr>
<tr>
<td>Te—O (equatorial)</td>
<td>1.88 Å (2x)</td>
<td>1.88 Å</td>
<td>1.88 Å</td>
<td>1.88 Å</td>
</tr>
<tr>
<td>( O_{ax} )-Te—O(_{ax})</td>
<td>168.0°</td>
<td>168.9°</td>
<td>147.8°</td>
<td>154.3°</td>
</tr>
<tr>
<td>( O_{eq} )-Te—O(_{eq})</td>
<td>100.6°</td>
<td>101.0°</td>
<td>100.0°</td>
<td>98.1°</td>
</tr>
</tbody>
</table>

The co-ordination of tellurium can be described in terms of a distorted trigonal bipyramid, in which one of the equatorial positions is unoccupied (cf. Fig. 2 and Table 6). This type of Te(IV) co-ordination has also been found in Te₂O₄·HNO₃,¹⁰ α-TeO₂,¹¹ and β-TeO₂,¹² and a comparison of bond distances and angles is given in Table 8. This co-ordination might be explained, as suggested by Pauling,¹³ and also pointed out by Beyer et al.,¹² in terms of a 5s5p²5d hybrid with an unshared electron pair occupying one of its equatorial orbitals. Swink and Carpenter¹⁰ have considered the equatorial bonds to be formed from the 5s, 5p₃, and 5p₄ orbitals and the axial bonds from the 5p₄ and 6s orbitals of the tellurium atom.

There is, however, no need to involve the doubtful 5d or 6s orbitals of the tellurium atom in bonding, if the equatorial bonds are considered to arise through the combination of the 5s, 5p₃, and 5p₄ atomic orbitals of tellurium, and if the axial molecular orbitals involve only the 5p₄ orbital of the tellurium atom and the p₄ orbitals of O₁ and O₄. Three different axial molecular orbitals are thus possible:

1. $p₄(\text{Te}) - (p₄(\text{O₁}) + p₄(\text{O₄}))$ — bonding orbital
2. $p₄(\text{Te}) + (p₄(\text{O₁}) - p₄(\text{O₄}))$ — non-bonding orbital
3. $p₄(\text{Te}) + (p₄(\text{O₁}) + p₄(\text{O₄}))$ — anti-bonding orbital.

Since there are 10 electrons available to fill the molecular orbitals, and if a lone pair is assumed to exist in the equatorial position, the axial bonds are formed by one bonding and one non-bonding molecular orbital. This model of the electronic configuration is also in accordance with the fact that the axial bonds are weaker than the equatorial bonds (cf. Table 8).

In Te(C₆H₄O₂)₂ the Te—O₁ bond is not significantly longer than the equatorial bonds. If, however, a weak interaction was assumed to exist between O₄ and the unshared electron pair of the tellurium atom in the neighbouring molecule, O₄ would not contribute to the axial molecular bond as much as O₁.

The effect of lone-pair-bond-pair repulsion¹⁴ may be seen in all of the structures cited in Table 8. In Te(C₆H₄O₂)₂ this distortion is more accentuated than in α-TeO₂ and β-TeO₂, and might perhaps be attributed to steric hindrance caused by the fixed O—O distance of approximately 2.6 Å in the catecholate groups.

No significant differences have been found in the bond distances and angles of the catecholate groups (cf. Table 7) as compared with those of catechol.¹⁵ The mean C—C bond distance in the carbon ring containing C₁—C₈ is 1.389 Å and the mean C—O distance is 1.373 Å, while the corresponding values in the other ring are 1.401 Å and 1.375 Å, respectively. These values are the same within the standard deviations as those found in catechol: 1.385 Å (C—C) and 1.372 Å (C—O).

There are no significant deviations of the carbon atoms from the best least squares plane through the actual rings (cf. Table 5). The tellurium atom is situated approximately in the plane defined by one of the catecholate groups, but is at a distance of 0.37 Å from the plane through the catecholate.
TELLURIUM(IV) CATECHOLATE

group containing \(O_4\). This difference between the two catecholate groups also supports the assumption that there is a weak intermolecular bond between \(O_4\) and Te.

During the course of this investigation, it was pointed out to me that a similar compound, \(K[As(C_8H_4O_3)_{2}]\), had recently been solved. In this structure \(As(III)\) shows a similar \(Me-O\) arrangement to that observed for Te(IV) in \(Te(C_8H_4O_3)_{2}\), but the trigonal bipyramid in \(K[As(C_8H_4O_3)_{2}]\) is slightly less distorted, the angle between the axial bonds being 166.2° and that between the two occupied equatorial bonds being 101.5°. In the arsenic compound there is, in distinction from \(Te(C_8H_4O_3)_{2}\), a clear difference between axial and equatorial bond lengths, i.e. 1.997 Å and 1.943 Å (axial) and 1.805 Å and 1.809 Å (equatorial). No intermolecular bond corresponding to that observed in \(Te(C_8H_4O_3)_{2}\) has, however, been found in \(K[As(C_8H_4O_3)_{2}]\).

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