# *m*-Iodobenzoic Acid Complexes with Selected Metals: Molecular Structure and Antimicrobial Activity

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Complexes of lithium, sodium, potassium, rubidium, cesium, magnesium, calcium, manganese, and zinc with *m*-iodobenzoic acid were studied. The FT-IR and FT-Raman spectra of the mentioned compounds in the solid state and water solutions were recorded and analyzed. Principal component analysis (PCA) was performed on the wavenumbers of selected bands (eight bands) occurring in the vibrational spectra. The numbers obtained as a result of this procedure characterize the electronic properties of the molecule of each complex. The antimicrobial activity of the studied compounds against selected bacteria (*Escherichia coli* and *Bacillus subtilis*) and yeast (*Saccharomyces cerevisiae* and *Hansenula anomala*) was estimated. The relationship between the chemical properties (as characterized by PCA of the IR spectra) and antimicrobial properties of the compounds was examined, and a good correlation between the two factors was found.

## INTRODUCTION

Various metal complexes (*1*) as well as benzoic acid and some of its derivatives show antimicrobial activity and are commonly used as food preservatives (*2–5*). The effect of various metal ions on the foodborne bacteria and yeast depending on ion concentration, its radius, and electronic properties is reported (*6, 7*). Hence, *m*-iodobenzoic acid complexes with selected metals are potential new preservative compounds, which, to our knowledge, have not been studied before.

In the literature the chemical compounds are characterized using principal component analysis (PCA) performed on the data of their vibrational spectra (*8, 9*). In such cases the electronic properties of the molecule are represented by one or more numbers. So far, there have been no reports that correlate the principal component of the compound with its antimicrobial activity. In some papers the relationship between the antimicrobial activity of some preservatives and the wavenumber of a selected single IR band is investigated (*6*). One band, even a very characteristic one, does not reflect the electronic properties of the whole molecule. The aim of this paper is to find out if there is any correlation between the electronic structure of the molecule (characterized by the first principal component) and its antimicrobial properties. Furthermore, such a new attempt is an opportunity to find the parameter that might be used as a sensor indicating

antimicrobial properties of the newly synthesized compounds being benzoic acid derivatives.

Water-soluble components offer better chances of practical application, so all of the compounds studied in this paper are water soluble.

## MATERIALS AND METHODS

The complexes of alkaline metals and calcium were prepared by dissolving appropriate *m*-iodobenzoic acid (Sigma analytical reagents) in an aqueous solution of metal hydroxide (Merck analytical reagent) in a stoichiometric ratio. Next, water was evaporated at 90 °C in a dryer. Then complex was dissolved and crystallized from the demineralized water. After drying, elementary analysis was performed. It showed that the ratio of metal to carboxylic anion was 1:1 in the case of alkaline metals and 1:2 in the case of calcium. Mg, Mn, and Zn complexes were obtained by mixing aqueous solutions of barium *m*-iodobenzoate (which were obtained in the same way as calcium *m*-iodobenzoate) with aqueous solutions of metal sulfates in a stoichiometric ratio. The barium sulfate was precipitated and separated. Next, water was evaporated from the solution at 90 °C in a dryer. The obtained complex was again dissolved and crystallized from demineralized water. The elementary analysis showed no evidence of the barium in the samples and the ratio of metal to carboxylic anion was 1:2.

Pressed KBr pellets were used for IR measurements within the range of 400–4000 cm$^{-1}$ with a Perkin-Elmer System 2000 FT-IR spectrometer. The water solution samples were measured using Perkin-Elmer ATR accessory. Raman spectra of solid state samples in capillary tubes were recorded within the range of 400–4000 cm$^{-1}$ with an FT-NIR Raman accessory of a Perkin-Elmer System 2000.

Two species of bacteria, *Escherichia coli* and *Bacillus subtilis*, as well as two species of yeasts, *Saccharomyces cerevisiae* and *Hansenula anomala*, were used for antimicrobial tests. Cultures of bacteria were maintained on broth medium at 37 °C for 24 h and then stored at 4 °C (*10*). Cultures of yeast were maintained on YDP medium at 28 °C for 2 days and then stored at 4 °C (*11*). Subcultures have been grafted into medium once each month.

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**Table 1. Wavenumbers and Intensities of Selected Bands Occurring in the IR and Raman Spectra of Complexes of Alkali Metals with *m*-Iodobenzoic Acids[a]**

| lithium *m*-iodobenzoate | | | | sodium *m*-iodobenzoate | | | | potassium *m*-iodobenzoate | | | | rubidium *m*-iodobenzoate | | | | cesium *m*-iodobenzoate | | | | assignment |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| IR | | Raman | | IR | | Raman | | IR | | Raman | | IR | | Raman | | IR | | Raman | | |
| 1590 | vs | 1587 | s | 1593 | vs | 1587 | vs | 1595 | vs | | | 1594 | vs | | | 1590 | vs | | | 8 b |
| 1579 | vs | 1552 | w | 1581 | vs | | | 1585 | sh | 1587 | s | 1583 | sh | 1583 | m | 1581 | sh | 1581 | m | 8 a |
| 1537 | vs | | | 1548 | vs | 1556 | m | 1551 | vs | 1549 | w | 1551 | vs | 1551 | w | 1548 | vs | 1544 | m | $\nu_{asym}(COO^-)$ |
| 1471 | w | 1472 | w | 1469 | w | 1469 | w | | | 1465 | w | | | 1466 | w | | | 1464 | w | 19 b |
| 1416 | vs | 1421 | w | 1412 | vs | 1423 | m | 1407 | s | 1412 | m | 1406 | vs | 1414 | m | 1406 | s | 1410 | vw | 19 a |
| 1399 | s | 1405 | vw | 1398 | vs | 1404 | w | 1387 | vs | 1392 | w | 1387 | vs | 1382 | m | 1386 | vs | 1380 | m | $\nu_{sym}(COO^-)$ |
| 1165 | w | 1171 | w | | | 1168 | vw | 1168 | vw | 1167 | w | 1168 | vw | 1168 | vw | 1167 | vw | 1165 | vw | 9 a |
| 1139 | w | 1146 | vw | 1138 | m | 1139 | w | 1134 | w | 1135 | w | 1134 | w | 1132 | vw | 1133 | w | 1128 | vw | 9 b |
| 1099 | m | 1089 | w | 1097 | w | | | 1082 | w | 1083 | vw | 1083 | w | | | 1083 | vw | | | 18 b |
| 1055 | m | 1060 | w | 1056 | m | 1058 | w | 1054 | w | 1056 | w | 1054 | w | 1055 | w | 1054 | vw | 1054 | vw | 18 a |
| 863 | m | 861 | vw | 854 | m | 858 | w | 850 | m | 852 | m | 849 | m | 856 | vw | 848 | v | 848 | vw | $\beta_{sym}(COO^-)$ |
| 747 | s | | | 751 | s | | | 761 | vs | | | 765 | s | | | 766 | s | | | $\gamma_{sym}(COO^-)$ |
| 707 | m | 712 | vw | 706 | m | 712 | m | 702 | m | 704 | w | 701 | m | 700 | w | 701 | w | 703 | w | 6 b |
| 542 | m | | | 532 | m | | | 528 | w | 526 | vw | 528 | w | | | 535 | w | | | $\beta_{asym}(COO^-)$ |
| 409 | w | | | 406 | m | | | 398 | w | 397 | w | 396 | w | 402 | vw | 395 | w | 397 | vw | 6 a |

[a] vs, very strong; s, strong; m, medium; w, weak; vw, very weak; sh, shoulder; $\nu$, stretching; $\beta$, in plane deformations; $\gamma$, out of plane deformations.

**Table 2. Wavenumbers and Intensities of Selected Bands Occurring in the IR and Raman Spectra of Complexes of Mg, Ca, Mn, and Zn with *m*-Iodobenzoic Acids[a]**

| magnesium *m*-iodobenzoate | | | | calcium *m*-iodobenzoate | | | | manganese *m*-iodobenzoate | | | | zinc *m*-iodobenzoate | | | | assignment |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| IR | | Raman | | IR | | Raman | | IR | | Raman | | IR | | Raman | | |
| 1591 | vs | 1589 | vs | 1592 | s | 1588 | vs | 1588 | s | 1588 | vs | 1590 | s | 1587 | vs | 8 b |
| 1581 | vs | | | 1580 | s | | | 1577 | s | | | 1575 | s | | | 8 a |
| 1542 | vs | 1539 | w | 1547 | vs | 1553 | w | 1539 | vs | | | 1536 | vs | 1531 | w | $\nu_{asym}(COO^-)$ |
| 1475 | w | 1475 | w | 1473 | w | 1471 | w | 1472 | w | 1474 | w | 1475 | w | 1479 | w | 19 b |
| 1438 | s | 1445 | w | 1421 | w | 1431 | m | 1419 | vs | 1438 | w | 1422 | vs | 1429 | w | 19 a |
| 1400 | s | 1395 | w | 1396 | vs | 1399 | w | 1389 | s | 1406 | w | 1396 | vs | 1399 | w | $\nu_{sym}(COO^-)$ |
| 1170 | vw | 1174 | vw | 1171 | vw | 1171 | vw | | | 1169 | vw | 1169 | vw | 1170 | vw | 9 a |
| 1144 | vw | 1146 | vw | 1144 | vw | 1144 | vw | 1143 | vw | | | 1143 | vw | 1142 | vw | 9 b |
| 1106 | vw | | | 1104 | vw | | | 1108 | w | | | | | | | 18 b |
| 1059 | w | 1059 | w | 1058 | w | 1057 | w | 1060 | w | 1060 | w | 1060 | w | 1060 | w | 18 a |
| 861 | vw | 862 | vw | 860 | w | 860 | w | 856 | w | 858 | w | 866 | vw | 866 | w | $\beta_{sym}(COO^-)$ |
| 752 | vs | | | 756 | vs | | | 756 | vs | | | 760 | vs | 763 | vw | $\gamma_{sym}(COO^-)$ |
| 706 | w | 708 | w | 709 | m | 710 | w | 703 | s | 708 | w | 709 | w | | | 6 b |
| 554 | vw | | | 545 | w | | | 550 | w | | | 567 | vw | | | $\beta_{asym}(COO^-)$ |
| 418 | vw | | | 418 | w | 409 | w | 411 | w | | | | | | | 6 a |

[a] vs, very strong; s, strong; m, medium; w, weak; vw, very weak; sh, shoulder; $\nu$, stretching; $\beta$, in plane deformations; $\gamma$, out of plane deformations.

The control flasks containing appropriate media were inoculated from cultures of tested microorganisms, and the final pH was made 7.4 for bacteria and 5.6 for yeast. The experimental flasks containing appropriate media were inoculated from cultures of tested microorganisms, and the tested chemical compound was added. The final concentration of tested complex was 0.15% for bacteria and 0.075% for yeast. The final pH of experimental samples was the same as in the controls. Three replicates were done for each inoculation.

The growth-inhibitor activity of *m*-iodobenzoic acid (treated as the reference) and *m*-iodobenzoates was estimated by comparing control (optimal conditions for microorganisms growth) and experimental (with tested compound) samples. The degree of inhibition of cell growth (in percents) was expressed as the difference between the number of colonies in control and experimental samples, divided by the number of colonies in the control.

All statistical calculations were done using the STAT-GRAPHICS Plus 2.1 package working on a Windows 98 platform.

## RESULTS AND DISCUSSION

The chemical composition of the compounds obtained in this work was estimated by elementary analysis (for example, the elementary analysis for sodium *m*-iodo-benzoate showed % C = 31.11; % O = 11.85; % H = 1.48;

55.56% for sodium and iodine). The characteristic bands occurring in the IR spectra of complexes (carboxylic anion bands, for example), which do not exist in the spectra of free acids, as well as the lack of some other bands which are characteristic for free acids (the C=O band, for example) show that the metal ion is connected to the carboxylic anion. This observation was made for both solid state and water solution samples. Along with the literature data (*12–14*), the appearance of the mentioned bands as well as the disappearance of others during the complexation reaction is proof that exchange of hydrogen by the metal ion takes place.

The series of nine compounds was studied. In this series the changing factor was the metal ion connected to the carboxylic anion. The vibrational spectra of the synthesized complexes were recorded and assigned. Tables 1 and 2 contain wavenumbers and intensities of the bands occurring in FT-IR and FT-Raman spectra of the studied complexes. $\nu$ indicates stretching, $\beta$, in plane deformations, and $\gamma$, out of plane deformations. The assignment was done on the basis of literature data (*12*, *13*) and our previous semiempirical calculations (*14*). The bands in the Tables 1 and 2 are numbered along with the notation used by Green (*15*, *16*) and

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**Table 3. First Principal Components (PC) of Studied Complexes**

| | metal ion | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | Li | Na | K | Rb | Cs | Mg | Ca | Mn | Zn |
| first PC | −1.49 | 0.79 | 3.26 | 2.30 | 1.79 | −0.33 | −1.76 | −1.20 | −3.35 |

Versanyi (*12*). In the first attempt the change of the wavenumber of a single selected band along with the change of the metal ion in the molecule was investigated. The wavenumber of the bands varied in the series Li → Cs. Some of them decreased [viz., $\nu_{sym}(COO^-)$ and $\beta_{sym}(COO^-)$] and some increased [viz., $\gamma_{sym}(COO^-)$], whereas others scattered [viz., $\nu_{asym}(COO^-)$ and $\beta_{asym}(COO^-)$]. The wavenumber of bands representing vibrations of the aromatic ring varied toward the series of metal ion (viz., 8a, 8b, 19a, and 19b). Principal component analysis (PCA) was performed to better describe the vibrational structure of the molecule and the change of the electronic properties of complexes along with the metal ion. The wavenumbers of the bands 8a, 8b, 19a, 19b, $\nu_{asym}(COO^-)$, $\nu_{sym}(COO^-)$, $\beta_{asym}(COO^-)$, and $\beta_{sym}(COO^-)$ were selected as data for the statistical procedure. Four of those bands reflect normal vibrations of the aromatic ring (8a, 8b, 19a, and 19b), whereas four of them reflect normal vibrations of the carboxylic anion $\nu_{asym}(COO^-)$, $\nu_{sym}(COO^-)$, $\beta_{asym}(COO^-)$, and $\beta_{sym}(COO^-)$. All of the selected bands are characteristic and occur in the spectrum of every studied complex. Furthermore, those bands are present in the spectra of water solutions. We believe, that this selection represents the vibrations of the whole molecule. The linear combination of wavenumbers of selected bands reflects the electronic properties of the whole molecule, which determine macroscopic properties of the compound (chemical reactivity, solubility, melting point, antimicrobial properties, and so on). The first principal components as the result of the PCA are gathered in the Table 3. The second and rest of the principal components were not statistically significant (the eigenvalues for them were <1.0) and are not presented. The first principal component accounts for 91.26% of the variability of the data set. Every studied complex has one number, and this number is treated as a numeric parameter that characterizes the change of the electronic charge distribution in the whole molecule along with the change of the metal ion. The PCA is known in the literature (*17*) as a statistical technique used for finding characteristic parameters of substances being in one series.

In the microbiological part, the growth-inhibitor activity of the *m*-iodobenzoic acid and studied complexes toward bacteria (*E. coli* and *B. subtilis*) and yeast (*S. cerevisiae* and *H. anomala*) was estimated. Table 4 contains the data reflecting the degree of growth inhibition observed after 24 h of incubation. The values in this table (between 0 and 100%) describe the degree of growth inhibition. The zero value would mean that there was no influence of the complex on the growth of

bacteria or yeast. This value was found for the reference *m*-iodobenzoic acid (it is not in the Table) for all studied microorganisms. This acid dissolves very poorly in water, and all microbial tests were carried out for saturated solutions (~0.002%). A value of 100 would mean that the complex totally inhibits the growth of microorganism.

The influence of the studied compounds on the growth of each studied microorganism varies depending on the metal ion. The influence of *m*-iodobenzoates on *E. coli* growth varies from 1 to 98%. The rubidium and cesium complexes show strong effects, whereas the Mg, Ca, Mn, and Zn complexes inhibit *E. coli* very weakly. In the case of *B. subtilis* three compounds (Li, Rb, and Cs complexes) exhibit strong inhibitory effects. On the other hand, calcium iodobenzoate inhibits *B. subtilis* only at 21%. The rest of compounds inhibit these bacteria on levels from 30 (Mn complex) to 84% (Na complex). The effects of the studied *m*-iodobenzoates on the *H. anomala* differ. The Rb complex inhibits this yeast at 99% and the Cs complex at 97%, whereas the Ca complex at only 12%. The other complexes influence the growth of *H. anomala* from 27% (zinc iodobenzoate) to 80% (potassium iodobenzoate). The effect of alkaline metal complexes on *S. cerevisiae* is relatively high (from 92% for K to 98% for Rb). The other compounds inhibit *S. cerevisiae* from 22 (Ca complex) to 68% (Mg complex). The alkaline metal complexes inhibit the growth of tested microorganisms to a higher degree (up to 98%) than bivalent ion complexes (up to 70%). However, there is no clear regularity toward metal series. This might suggest that the kind of metal ion is not the only factor which determines the antimicrobial activity of the compound. This suggestion is confirmed by the observation that there is a relationship between the antimicrobial activity and the first principal component (for this analysis, the wavenumber of the bands of aromatic ring vibration were taken).

Among all of the studied compounds Rb and Cs complexes exhibit the highest activity against tested bacteria and yeast. The Cs complex is particularly interesting, as its toxicity against each microorganism is 97−98%.

An attempt was made to find the relationship between the antimicrobial activity of each compound and the wavenumber of the selected single band occurring in the spectrum. The aim was to find the band that might be the "diagnostic" one. The wavenumber of the diagnostic band would be connected with antimicrobial activity. Unfortunately, the correlation of the wavenumber of some single bands and the antimicrobial activity of the compounds was poor, statistically not significant.

In our opinion, in the case of the studied complexes the whole molecule of each compound is responsible for the inhibitory effect. Furthermore, we believe that there exists a relationship between the antimicrobial activity of complex and its first principal component, which is a measure of the electronic properties of whole molecule.

**Table 4. Degree of Growth Inhibition of *E. coli*, *B. subtilis*, *H. anomala*, and *S. cerevisiae* Caused by the Studied Complexes (Percent)[a]**

| microorganism | Li | Na | K | Rb | Cs | Mg | Ca | Mn | Zn |
|---|---|---|---|---|---|---|---|---|---|
| *E. coli* | 39 ± 3.60 | 32 ± 3.60 | 29 ± 3.00 | 90 ± 5.56 | 98 ± 1.73 | 6 ± 2.65 | 8 ± 1.73 | 11 ± 1.00 | 1 ± 1.00 |
| *B. subtilis* | 90 ± 5.29 | 84 ± 5.29 | 80 ± 4.36 | 90 ± 2.65 | 98 ± 1.00 | 50 ± 5.29 | 21 ± 3.60 | 30 ± 3.46 | 50 ± 4.36 |
| *H. anomala* | 77 ± 6.11 | 64 ± 7.81 | 80 ± 7.37 | 99 ± 1.00 | 97 ± 1.73 | 38 ± 2.00 | 12 ± 2.05 | 56 ± 2.65 | 27 ± 4.36 |
| *S. cerevisiae* | 90 ± 2.64 | 95 ± 2.00 | 92 ± 4.00 | 98 ± 1.00 | 97 ± 1.00 | 68 ± 4.36 | 22 ± 2.65 | 45 ± 3.00 | 26 ± 1.73 |

[a] Presented values are means of three measurements.

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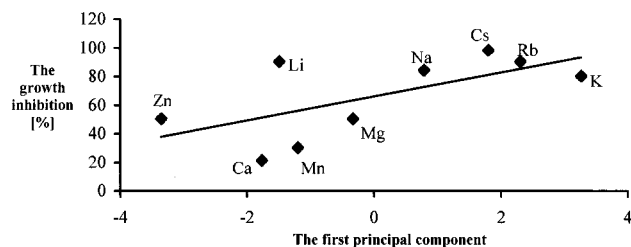


**Figure 1.** Relationship between the first principal components of the studied complexes and their antimicrobial activities (the means of three measurements) against *B. subtilis.*

An attempt was made to find the correlation between those two parameters. Figure 1, for example, presents the linear correlation between the activity of the studied *m*-iodobenzoates against *B. subtilis* and their first principal components. In this case the correlation coefficient is equal to −0.82. A similar relationship exists for other tested microorganisms as well. The correlation coefficients are −0.81 for *E. coli*, −0.83 for *H. anomala*, and −0.80 for *S. cerevisiae*. For all correlations the *p* values in the ANOVA tables were <0.05, which means the relationships are statistically significant at the 95% confidence level. Furthermore, the results of fitting some curvilinear models (exponential, square root *y*, reciprocal *y*, reciprocal *x*, double reciprocal, logarithmic *x*, mulitiplicative, square root *x*, *s* curve, and logistic log probit) were compared. Comparison of alternative models showed highest correlation coefficients for the linear model.

It may be asked why complexes of the mono- and bivalent metal ions were gathered in the same group. The point is that the bands representing the same vibrations occur in every spectrum (both mono- and bivalent ion complexes) and the increase of the number of the data involved in the PCA produces more accurate results. Therefore, the change of the electronic properties of the molecule toward the series of metals is properly described using only one parameter. Furthermore, the results obtained show that this attempt was correct, as the found correlation (where all metal ions are together) is high.

FINAL REMARKS

It is important that most of the studied compounds show antimicrobial activity. Some of them (especially the Cs complexes) are active against all of the studied microorganisms. The correlation analysis confirmed that antimicrobial activity depends on the electronic properties of the whole molecule. A relationship was found between the first principal component and antimicrobial activity. On the other hand, there was no correlation between a single band wavenumber and antimicrobial activity. Had such a correlation occurred, this would have suggested that only a part of the molecule (for example, the aromatic ring or carboxylic anion) is responsible for the inhibition of the growth of microorganisms. The metal ion determines antimicrobial properties in a special way, by changing the electronic charge distribution in the whole molecule. The mechanisms of metal influence on the aromatic ring are explained in the literature: disturbances in the aromatic system involve either polarization of bonds by the appearance of or increase in partial positive and negative charges on adjacent carbon atoms in the ring or an increase in

the dipole moment of a molecule as a whole (*18*, *19*). The described relationship suggests that the PCA based on the spectroscopic (FT-IR) data might be useful in preliminary analyses of the antimicrobial properties of series of compounds. The first principal component, which describes the electronic charge distribution in the molecule, might be useful for selection among newly synthesized compounds to find those that offer better chances for antimicrobial activity. Microbiological tests are more time-consuming as compared to spectroscopic measurement and statistical procedure, and there is no need to perform those tests for every compound. If a newly synthesized compound belongs to the series of which the antimicrobial activity is estimated, one might predict the properties of a new compound and decide if microbial tests are necessary. Our concept is quite new and needs to be confirmed using other series of compounds.

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