Electronic Absorption
and Internal and External
Vibrational Data of
Atomic and Molecular Ions
Doped in Alkali Halide
Crystals
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2 Part of the Center for Radiation Research.
3 Located at Boulder, Colorado 80302.
4 Part of the Center for Building Technology.
Electronic Absorption and
Internal and External Vibrational Data of Atomic
and Molecular Ions Doped in Alkali Halide Crystals

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and S. K. Agarwal

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Foreword

The National Standard Reference Data System provides access to the quantitative data of physical science, critically evaluated and compiled for convenience and readily accessible through a variety of distribution channels. The System was established in 1963 by action of the President's Office of Science and Technology and the Federal Council for Science and Technology, and responsibility to administer it was assigned to the National Bureau of Standards.

NSRDS receives advice and planning assistance from a Review Committee of the National Research Council of the National Academy of Sciences-National Academy of Engineering. A number of Advisory Panels, each concerned with a single technical area, meet regularly to examine major portions of the program, assign relative priorities, and identify specific key problems in need of further attention. For selected specific topics, the Advisory Panels sponsor subpanels which make detailed studies of users' needs, the present state of knowledge, and existing data resources as a basis for recommending one or more data compilation activities. This assembly of advisory services contributes greatly to the guidance of NSRDS activities.

The System now includes a complex of data centers and other activities in academic institutions and other laboratories. Components of the NSRDS produce compilations of critically evaluated data, reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data. The centers and projects also establish criteria for evaluation and compilation of data and recommend improvements in experimental techniques. They are normally associated with research in the relevant field.

The technical scope of NSRDS is indicated by the categories of projects active or being planned: nuclear properties, atomic and molecular properties, solid state properties, thermodynamic and transport properties, chemical kinetics, and colloid and surface properties.

Reliable data on the properties of matter and materials is a major foundation of scientific and technical progress. Such important activities as basic scientific research, industrial quality control, development of new materials for building and other technologies, measuring and correcting environmental pollution depend on quality reference data. In NSRDS, the Bureau's responsibility to support American science, industry, and commerce is vitally fulfilled.

Richard W. Roberts, Director
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Electronic Absorption and Internal and External Vibrational Data of Atomic and Molecular Ions Doped in Alkali Halide Crystals

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Department of Physics
Indian Institute of Technology
New Delhi 110029, India

Spectral data for more than 70 atomic and molecular ions doped in alkali halide crystals are tabulated. The tables include electronic absorption data, listings of internal vibrational frequencies of doped complex ions, and tabulations of the frequencies of external modes. The data that appear in the tables were selected on the basis of the consistency among different authors, the types of instruments, and the temperature of measurement. In addition to the data, the tables include the spectroscopic assignments given by the authors in the references cited.

Key words: Atomic ions; doped alkali halide crystals; external vibrational modes; internal vibrational modes; molecular ions.

Introduction

When atomic and molecular impurity ions are doped in crystals, the optical (electronic) absorption spectrum of the ions will be modified. Because of the low symmetry of the environment (lower than spherical symmetry), the degeneracies of free ion levels can split and transitions between these split levels can take place. These transitions give rise to the so-called crystal field bands and can be interpreted on the basis of crystal field theory [1]. In addition, transitions involving the transfer of charge between the impurity ion and the surrounding ligands also can occur, giving rise to strong charge transfer absorption bands. If there is considerable overlap of the wave functions of the impurity ion and the ligands, further modifications of the spectra occur due to covalency effects, and the observed spectra can only be explained on the basis of ligand field theory and molecular orbital theory [2, 3]. Thus the study of optical absorption spectra gives information about the symmetry of the crystal field as well as the nature of the interaction between the impurity ion and the host lattice. The crystal field transitions are parity forbidden and they are phonon assisted. Temperature dependence of the optical spectrum gives the nature of the transitions.

Complex molecular ions, in addition to their electronic spectrum, give infrared and Raman spectra due to their internal vibrational modes [4, 5]. When such ions are doped in crystals, their vibrational frequencies shift depending upon the size of the host lattice sites and of the complex ion as well as the interaction between the ions [6]. Splitting of the degenerate vibrational modes may occur due to lowering of the symmetry of the ion whenever defects are present in the nearest or next nearest neighbour positions [7, 8]. These internal vibrational modes can sometimes show side bands due to combination with the external modes of impurity host lattice system [9, 10]. Therefore, a detailed study of the internal vibrational modes of molecular impurities gives useful information about the defect properties as well as the phonon spectrum of the host lattice.

When impurity ions are introduced into a lattice, new modes are induced in the lattice giving rise to an absorption spectrum in the far infrared. If the impurity is monoatomic, only localized, resonant, or gap modes are induced, depending upon whether the new absorption appears above the optical band, in the acoustic continuum, or in the gap between the acoustic and optical branches, respectively [11]. Whether the impurity will induce a localized, resonant, or gap mode will depend upon the relative mass of the impurity ion with respect to the ion it replaces, as well as the force constant between the impurity and the host lattice ions. If, on the other hand, the impurity is molecular, in addition to these modes, librational as well as tunneling modes are also induced [7, 12]. These new modes can give rise to far infrared absorption and Raman scattering, and show strong resonant scattering of phonons in thermal conductivity. Impurity also breaks down the

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** Present address: Solid State Physics Laboratory, Lucknow Road, Delhi 110007, India.
1 Figures in brackets indicate literature references on page 2.
translational symmetry of the lattice, and vibrations at all points in the Brillouin zone become infrared and/or Raman active depending upon the symmetry of the mode. Thus impurity induced infrared and Raman spectra can be used to map the phonon spectrum of the host lattice.

Alkali halide crystals doped with more than 70 different impurity ions have been investigated from the above-mentioned points of view [13]. This is because of the ease with which pure and well-characterized alkali halide crystals can be grown, as well as to their almost perfect ionic nature, precise knowledge of the location of the ions and the neighbouring defect in the lattice, etc. The cubic symmetry of the crystal field and the exact knowledge of the symmetry of the field due to defects in the vicinity of the impurity ion, make alkali halides excellent hosts to study and to interpret the optical and other defect sensitive properties of ions.

In alkali halide crystals most of the impurities enter substitutionally at the cation or anion site depending upon whether the impurity is cationic or anionic, respectively. In the case of a few large complex impurity ions such as Co(CN)_6, Fe(CN)_6, etc., the impurity replaces a complex group of seven lattice sites MX_6 (M—an alkali ion and X—a halide ion). If the impurity is divalent, extra charge is compensated by the creation of vacancies or by intentionally doped or background charge compensating impurity ions. The symmetry of the environment about the Co(CN)_6 group is determined by the location of the charge compensating entity.

Impurity doped alkali halides find many modern technological applications. Tl⁺ doped NaI is a well known scintillator and is extensively used in γ-ray scintillation counters. Color centers in alkali halides are being used successfully as memory devices. Recently it has been shown that the paraelectric property of Li⁺ in KCl can be used as a thermometer to measure extremely low temperatures.

With the wide academic interest and potential technological applications of impurity centers in alkali halides, the availability of comprehensive optical data of different centers in alkali halide crystals is extremely valuable. The amount of literature on the optical properties of impurity centers in alkali halides has grown so much in the last ten years that it is extremely difficult for one to keep track of the development. It is therefore desirable to gather all the optical data in one place for all the impurity centers doped in alkali halides so that this can serve as a ready reference.

The following tables on the optical properties have been prepared by critically going through more than 500 papers listed in [13] and other relevant papers published before 1964. The references are given for those papers from which the actual data reported is taken. If more than one paper exists on the same impurity ion, the data are evaluated on the basis of the experimental procedures used, the resolution and accuracy of the instruments employed for measurements, consistency of the data between different authors, and quality of the samples on which measurements were made. Assignments given for the absorption bands in the table are those reported in the references.

The reference data are divided into three parts. In Part I the electronic absorption bands are tabulated. Here the peak positions are given in nanometers (nm). The data given in eV in the paper are converted to nm using the relation 1 eV = 1239.0 nm. Wherever possible the temperature of measurement is also indicated for each band.

Since the available data on halfwidth/oscillator strength of the absorption bands are meager and not consistent among different authors, we have not included them.

The data on the internal vibrational frequencies of complex ions doped in alkali halide crystals are given in Part II. Here the frequencies are given in wavenumbers (cm⁻¹) and the ions are arranged in the order of increasing number of atoms in the complex ions.

In Part III the frequencies of the external modes are presented. Here again the frequencies are in wavenumbers (cm⁻¹). The data are presented first for monoatomic impurities and then for the molecular ions.

References are given at the end of each table.

References

* In keeping with commonly accepted conventions in molecular spectroscopy, certain energies have been expressed in their wavenumber (cm⁻¹) equivalents. The actual energy can be obtained by multiplying the cm⁻¹ equivalent by ħc.
PART I.

Electronic Absorption of Impurity Centers Doped in Alkali Halide Crystals
### Table 1. Optical absorption bands (in nm) of copper centers in alkali halides

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*Room temperature.

^Liquid air/nitrogen temperature.

^Liquid helium temperature.

^Temperature between 4.2 and 77 K.

**References**


### Table 2. Optical absorption bands (in nm) of silver centers in alkali halides

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* Room temperature.
* Liquid air/nitrogen temperature.
* Liquid helium temperature.
* Temperature between 4.2 and 77 K.

References

### Table 3. Optical absorption bands (in nm) of gold centers in alkali halides

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- a: Room temperature.
- b: Liquid air/nitrogen temperature.
- c: Liquid helium temperature.
- d: Temperature between 4.2 and 77 K.

### References


### Table 4. Optical absorption bands (in nm) of magnesium ions in alkali halides

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- a: Room temperature.
- b: Liquid air/nitrogen temperature.
- c: Liquid helium temperature.
- d: Temperature between 4.2 and 77 K.

### References


### Table 5. Optical absorption bands (in nm) of calcium centers in alkali halides

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- a: Room temperature.
- b: Liquid air/nitrogen temperature.
- c: Liquid helium temperature.
- d: Temperature between 4.2 and 77 K.

### References

### Table 6. Optical absorption bands (in nm) of strontium centers in alkali halides

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"aRoom temperature.  "bLiquid air/nitrogen temperature.  "cLiquid helium temperature.  "dTemperature between 4.2 and 77 K.

### References


### Table 7. Optical absorption bands (in nm) of barium centers in alkali halides

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"aRoom temperature.  "bLiquid air/nitrogen temperature.  "cLiquid helium temperature.  "dTemperature between 4.2 and 77 K.

### References


### Table 8. Optical absorption bands (in nm) of zinc centers in alkali halides

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"aRoom temperature.  "bLiquid air/nitrogen temperature.  "cLiquid helium temperature.  "dTemperature between 4.2 and 77 K.

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### Table 9. Optical absorption bands (in nm) of cadmium centers in alkali halides

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*Room temperature.

*Liquid air/nitrogen temperature.

*Liquid helium temperature.

*Temperature between 4.2 and 77 K.

### References


### Table 10. Optical absorption bands (in nm) of mercury centers in alkali halides

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*Room temperature.

*Liquid air/nitrogen temperature.

*Liquid helium temperature.

*Temperature between 4.2 and 77 K.

### References


Table 11. Optical absorption bands (in nm) of gallium centers in alkali halides.

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*Room temperature.
\(b\) Liquid air/nitrogen temperature.
\(c\) Liquid helium temperature.
\(d\) Temperature between 4.2 and 77 K.

References


Table 12. Optical absorption bands (in nm) of indium centers in alkali halides.

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*Room temperature.
\(b\) Liquid air/nitrogen temperature.
\(c\) Liquid helium temperature.
\(d\) Temperature between 4.2 and 77 K.

References

### Table 13. Optical absorption bands (in nm) of germanium centers in alkali halides

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* Room temperature.
* Liquid air/nitrogen temperature.

### References


### Table 14. Optical absorption bands (in nm) of bismuth centers in alkali halides

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* Room temperature.
* Liquid air/nitrogen temperature.

### References


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* Room temperature.
* Liquid air/nitrogen temperature.
* Liquid helium temperature.
* Temperature between 4.2 and 77 K.

**References**

### Table 16. Optical absorption bands (in nm) of tin centers in alkali halides

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a) Room temperature.
b) Liquid air/nitrogen temperature.
c) Liquid helium temperature.
d) Temperature between 4.2 and 77 K.

### References


### Table 17. Optical absorption bands (in nm) of lead centers in alkali halides

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13
### Table 17. Optical absorption bands (in nm) of lead centers in alkali halides—Continued

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<td>b 497</td>
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* Room temperature.
* Liquid air/nitrogen temperature.
* Liquid helium temperature.
* Temperature between 4.2 and 77 K.

**References**


### Table 18. Optical absorption bands (in nm) of titanium centers in alkali halides

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* Room temperature.
* Liquid air/nitrogen temperature.
* Liquid helium temperature.
* Temperature between 4.2 and 77 K.

**References**

### Table 19. Optical absorption bands (in nm) of vanadium centers in alkali halides

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$^a$ Room temperature.

$^b$ Liquid air/nitrogen temperature.

$^c$ Liquid helium temperature.

$^d$ Temperature between 4.2 and 77 K.

### References


### Table 20. Optical absorption bands (in nm) of chromium centers in alkali halides

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$^a$ Room temperature.

$^b$ Liquid air/nitrogen temperature.

$^c$ Liquid helium temperature.

$^d$ Temperature between 4.2 and 77 K.

### References


### Table 21. Optical absorption bands (in nm) of manganese centers in alkali halides

<table>
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Table 21. Optical absorption bands (in nm) of manganese centers in alkali halides—Continued

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* Room temperature.
* Liquid air/nitrogen temperature.
* Liquid helium temperature.
* Temperature between 4.2 and 77 K.

References


Table 22. Optical absorption bands (in nm) of cobalt centers in alkali halides

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 Table 22. Optical absorption bands (in nm) of cobalt centers in alkali halides—Continued

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References

Table 23. Optical absorption bands (in nm) of nickel centers in alkali halides

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*Room temperature.
*Liquid air/nitrogen temperature.
*Liquid helium temperature.
*Temperature between 4.2 and 77 K.

References


Table 24. Optical absorption bands (in nm) of rhodium centers in alkali halides

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*Room temperature.
*Liquid air/nitrogen temperature.
*Liquid helium temperature.
*Temperature between 4.2 and 77 K.

Reference


Table 25. Optical absorption bands (in nm) of palladium centers in alkali halides

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*Room temperature.
*Liquid air/nitrogen temperature.
*Liquid helium temperature.
*Temperature between 4.2 and 77 K.

References

Table 26. Optical absorption bands (in nm) of europium centers in alkali halides

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$^a$Room temperature.
$^b$Liquid air/nitrogen temperature.
$^c$Liquid helium temperature.
$^d$Temperature between 4.2 and 77 K.

References

Table 27. Optical absorption bands (in nm) of samarium centers in alkali halides

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### Table 27. Optical absorption bands (in nm) of samarium centers in alkali halides—Continued

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| Sm⁺    | ---  | --- | b1250 | --- | --- | --- | *H⁶/2 | [4]         |
|        | ---  | --- | b1120 | --- | --- | --- | *H⁷/2 | [4]         |
|        | ---  | --- | b961.6 | --- | --- | --- | *H⁹/2 | [4]         |
|        | ---  | --- | b861.1 | --- | --- | --- | *H₁₁/2 | [4]         |
|        | ---  | --- | b799.2 | --- | --- | --- | *H₁₂/2 | [4]         |

a Room temperature
b Liquid air/nitrogen temperature.
c Liquid helium temperature.
d Temperature between 4.2 and 77 K.

### References


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### Table 28. Optical absorption bands (in nm) of holmium centers in alkali halides

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<td>b269</td>
<td>b260</td>
<td>4f¹¹ → 4f¹⁰5d</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>b245</td>
<td>b225</td>
<td>4f¹¹ → 4f¹⁰5d</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>b234</td>
<td>b216</td>
<td>4f¹¹ → 4f¹⁰5d</td>
<td>[1]</td>
</tr>
<tr>
<td>Ho⁻</td>
<td>---</td>
<td>a375</td>
<td>---</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>---</td>
<td>a282</td>
<td>---</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>---</td>
<td>a252</td>
<td>---</td>
<td>[1]</td>
</tr>
<tr>
<td>Ho⁺⁺</td>
<td>---</td>
<td>a220</td>
<td>Clusters of Ho⁰</td>
<td>[1]</td>
</tr>
</tbody>
</table>

a Room temperature.
b Liquid air/nitrogen temperature.
c Liquid helium temperature.
d Temperature between 4.2 and 77 K.

### Reference

### Table 29. Optical absorption bands (in nm) of ytterbium centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>NaCl</th>
<th>KCl</th>
<th>KBr</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yb(^{2+})</td>
<td>b 270</td>
<td>b 270</td>
<td>---</td>
<td>b 230</td>
<td>[3]</td>
</tr>
<tr>
<td>Yb(^{3+})</td>
<td>b 270</td>
<td>b 270</td>
<td>---</td>
<td>---</td>
<td>[1]</td>
</tr>
</tbody>
</table>

\(\text{a}\) Room temperature.  
\(\text{b}\) Liquid air/nitrogen temperature.  
\(\text{c}\) Liquid helium temperature.  
\(\text{d}\) Temperature between 4.2 and 77 K.

**References**


### Table 30. Optical absorption bands (in nm) of uranyl centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>LiF</th>
<th>NaCl</th>
<th>KCl</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>UO(^{2+})</td>
<td>b 290</td>
<td>b 290</td>
<td>b 270</td>
<td>---</td>
<td>[1, 2]</td>
</tr>
</tbody>
</table>

\(\text{a}\) Room temperature.  
\(\text{b}\) Liquid air/nitrogen temperature.  
\(\text{c}\) Liquid helium temperature.  
\(\text{d}\) Temperature between 4.2 and 77 K.

**References**


### Table 31. Optical absorption bands (in nm) of hydrogen centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>NaF</th>
<th>NaCl</th>
<th>NaBr</th>
<th>NaI</th>
<th>KCl</th>
<th>KBr</th>
<th>KI</th>
<th>RbCl</th>
<th>RbBr</th>
<th>Rbl</th>
<th>CsBr</th>
<th>CsI</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>U(H(^{-}))</td>
<td>a 157</td>
<td>192</td>
<td>210</td>
<td>---</td>
<td>d 211.5</td>
<td>d 225</td>
<td>244</td>
<td>d 226</td>
<td>242</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>U(D(^{-}))</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>d 210.8</td>
<td>d 224</td>
<td>---</td>
<td>d 225.3</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>d 268.5</td>
<td>---</td>
</tr>
<tr>
<td>U(_1^+)</td>
<td>---</td>
<td>d 220</td>
<td>d 259</td>
<td>d 328</td>
<td>d 235</td>
<td>d 272</td>
<td>d 337</td>
<td>d 247</td>
<td>d 280.5</td>
<td>d 345</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>U(_1^+)</td>
<td>---</td>
<td>---</td>
<td>d 242.5</td>
<td>d 300</td>
<td>---</td>
<td>---</td>
<td>d 257</td>
<td>d 315</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>U(_2^+)</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>d 217</td>
<td>d 255.5</td>
<td>---</td>
<td>d 240.5</td>
<td>d 266.5</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
<td>---</td>
</tr>
</tbody>
</table>

\(\text{a}\) Room temperature.  
\(\text{b}\) Liquid air/nitrogen temperature.  
\(\text{c}\) Liquid helium temperature.  
\(\text{d}\) Temperature between 4.2 and 77 K.

**References**

Table 32. Optical absorption bands (in nm) of halogen centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>NaBr</th>
<th>KCl</th>
<th>KBr</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>I&lt;sup&gt;-&lt;/sup&gt;</td>
<td>b193.5</td>
<td>b184.7</td>
<td>b193.8</td>
<td>___</td>
<td>[1, 2]</td>
</tr>
</tbody>
</table>

<sup>a</sup>Room temperature.  <sup>b</sup>Liquid air/nitrogen temperature.  
<sup>c</sup>Liquid helium temperature.  <sup>d</sup>Temperature between 4.2 and 77 K.

References


Table 33. Optical absorption bands (in nm) of oxygen centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>NaF</th>
<th>NaCl</th>
<th>KCl</th>
<th>KBr</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>O&lt;sub&gt;2&lt;/sub&gt;</td>
<td>___</td>
<td>___</td>
<td>b248</td>
<td>b248</td>
<td>___</td>
<td>[1]</td>
</tr>
<tr>
<td>142</td>
<td>___</td>
<td>194</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>[2, 3]</td>
</tr>
</tbody>
</table>

<sup>a</sup>Room temperature.  <sup>b</sup>Liquid air/nitrogen temperature.  
<sup>c</sup>Liquid helium temperature.  <sup>d</sup>Temperature between 4.2 and 77 K.

References


Table 34. Optical absorption bands (in nm) of sulphur centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>KCl</th>
<th>KBr</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>SH&lt;sup&gt;-&lt;/sup&gt;</td>
<td>b185.1</td>
<td>b193.6</td>
<td>___</td>
<td>[1, 2, 3]</td>
</tr>
<tr>
<td>S&lt;sup&gt;-&lt;/sup&gt;</td>
<td>b192.4</td>
<td>b203.5</td>
<td>___</td>
<td>[1, 2, 3]</td>
</tr>
<tr>
<td>S&lt;sup&gt;2-&lt;/sup&gt;</td>
<td>b393.5</td>
<td>___</td>
<td>___</td>
<td>[2]</td>
</tr>
</tbody>
</table>

<sup>a</sup>Room temperature.  <sup>b</sup>Liquid air/nitrogen temperature.  
<sup>c</sup>Liquid helium temperature.  <sup>d</sup>Temperature between 4.2 and 77 K.

References


Table 35. Optical absorption bands (in nm) of selenium centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>KCl</th>
<th>KBr</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>SeH&lt;sup&gt;-&lt;/sup&gt;</td>
<td>d202.4</td>
<td>d211.4</td>
<td>___</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>d193.6</td>
<td>d202.3</td>
<td>___</td>
<td>[1]</td>
</tr>
<tr>
<td>Se&lt;sup&gt;-&lt;/sup&gt;</td>
<td>d208.6</td>
<td>d219.0</td>
<td>___</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>d201.6</td>
<td>d212.6</td>
<td>___</td>
<td>[1]</td>
</tr>
<tr>
<td>Se&lt;sup&gt;2-&lt;/sup&gt;</td>
<td>d395</td>
<td>d406.5</td>
<td>___</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>d364</td>
<td>d374</td>
<td>___</td>
<td>[1]</td>
</tr>
</tbody>
</table>

<sup>a</sup>Room temperature.  <sup>b</sup>Liquid air/nitrogen temperature.  
<sup>c</sup>Liquid helium temperature.  <sup>d</sup>Temperature between 4.2 and 77 K.

References

Table 36. Optical absorption bands (in nm) of OH/OD centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>NaF</th>
<th>NaCl</th>
<th>KCl</th>
<th>KBr</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>OH&lt;sup&gt;-&lt;/sup&gt;</td>
<td>151.2</td>
<td><em>b</em> 185</td>
<td><em>c</em> 205</td>
<td>b 214</td>
<td>___</td>
<td>[1. 2. 3. 4]</td>
</tr>
<tr>
<td>OD&lt;sup&gt;-&lt;/sup&gt;</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
<td>___</td>
</tr>
</tbody>
</table>

<sup>a</sup> Room temperature.  
<sup>b</sup> Liquid air/nitrogen temperature.  
<sup>c</sup> Liquid helium temperature.  
<sup>d</sup> Temperature between 4.2 and 77 K.

References


Table 37. Optical absorption bands (in nm) of amide centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>KCl</th>
<th>KBr</th>
<th>KI</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH&lt;sub&gt;2&lt;/sub&gt;</td>
<td>d 253.9</td>
<td>d 272.2</td>
<td>d 295.0</td>
<td>0–0</td>
<td>[1]</td>
</tr>
<tr>
<td>ND&lt;sub&gt;2&lt;/sub&gt;</td>
<td>d 251.8</td>
<td>d 268.5</td>
<td>d 294.0</td>
<td>0–0</td>
<td>[1]</td>
</tr>
</tbody>
</table>

<sup>a</sup> Room temperature.  
<sup>b</sup> Liquid air/nitrogen temperature.  
<sup>c</sup> Liquid helium temperature.  
<sup>d</sup> Temperature between 4.2 and 77 K.

References


Table 38. Optical absorption bands (in nm) of nitrite centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>NaBr</th>
<th>KCl</th>
<th>KBr</th>
<th>KI</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO&lt;sub&gt;2&lt;/sub&gt;</td>
<td><em>c</em> 397.2</td>
<td><em>c</em> 398.8</td>
<td><em>c</em> 401.1</td>
<td><em>c</em> 401.1</td>
<td>Zero-phonon transition</td>
<td>[1. 2]</td>
</tr>
</tbody>
</table>

<sup>a</sup>This band shows vibrational progression with separations (~ 1010 cm<sup>-1</sup> and 600 cm<sup>-1</sup>).  
<sup>b</sup>Liquid air/nitrogen temperature.  
<sup>c</sup>Liquid helium temperature.  
<sup>d</sup>Temperature between 4.2 and 77 K.

References


Table 39. Optical absorption bands (in nm) of chromate centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>KCl</th>
<th>KBr</th>
<th>KI</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>CrO&lt;sub&gt;4&lt;/sub&gt;&lt;sup&gt;2-&lt;/sup&gt;</td>
<td><em>b</em> 335</td>
<td><em>b</em> 355</td>
<td><em>b</em> 365</td>
<td>*t&lt;sub&gt;1&lt;/sub&gt;→e</td>
<td>[1. 2]</td>
</tr>
<tr>
<td></td>
<td>——</td>
<td><em>b</em> 285</td>
<td>——</td>
<td>——</td>
<td>[1. 2]</td>
</tr>
<tr>
<td></td>
<td><em>b</em> 270</td>
<td><em>b</em> 270</td>
<td><em>b</em> 270</td>
<td>*t&lt;sub&gt;1&lt;/sub&gt;→t&lt;sub&gt;2&lt;/sub&gt;</td>
<td>[1. 2]</td>
</tr>
<tr>
<td></td>
<td><em>b</em> 240</td>
<td><em>b</em> 246</td>
<td>——</td>
<td>——</td>
<td>[1. 2]</td>
</tr>
</tbody>
</table>

<sup>a</sup>This absorption band shows a vibrational progression with a separation of 800 cm<sup>-1</sup>. The peak position reported here corresponds to the strongest peak in the progression.  
<sup>b</sup>Liquid air/nitrogen temperature.  
<sup>c</sup>Liquid helium temperature.  
<sup>d</sup>Temperature between 4.2 and 77 K.

References

### Table 40. Optical absorption bands (in nm) of permanganate centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>KBr</th>
<th>KI</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnO(_2^+)</td>
<td><em>c</em> 600</td>
<td><em>c</em> 650</td>
<td>(t_1 \rightarrow e)</td>
<td>[1, 2]</td>
</tr>
<tr>
<td></td>
<td><em>c</em> 520</td>
<td><em>c</em> 540</td>
<td>(t_1 \rightarrow e)</td>
<td>[1, 2]</td>
</tr>
<tr>
<td></td>
<td><em>c</em> 390</td>
<td>----</td>
<td>(t_2 \rightarrow e)</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td><em>c</em> 336</td>
<td>----</td>
<td>(t_2 \rightarrow e)</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td><em>c</em> 305</td>
<td>----</td>
<td>----</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td><em>c</em> 230</td>
<td>----</td>
<td>(t_1 \rightarrow t_2)</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td><em>c</em> 200</td>
<td>----</td>
<td>----</td>
<td>[1]</td>
</tr>
</tbody>
</table>

*These bands show vibrational progression with separations of 760 cm\(^{-1}\) and 780 cm\(^{-1}\). The peak position corresponds to the strongest peak in the progression.

a Room temperature.
b Liquid air/nitrogen temperature.
c Liquid helium temperature.
d Temperature between 4.2 and 77 K.

**References**


### Table 41. Optical absorption bands (in nm) of manganate centers in alkali halides

<table>
<thead>
<tr>
<th>Center</th>
<th>KCl</th>
<th>KBr</th>
<th>KI</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>MnO(_2^+)</td>
<td><em>b</em> 850</td>
<td><em>b</em> 850</td>
<td><em>b</em> 850</td>
<td>(e \rightarrow t_2)</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td><em>b</em> 600</td>
<td><em>b</em> 600</td>
<td><em>b</em> 600</td>
<td>(t_1 \rightarrow e)</td>
<td>[1, 2]</td>
</tr>
<tr>
<td></td>
<td><em>b</em> 430</td>
<td><em>b</em> 430</td>
<td><em>b</em> 430</td>
<td>(t_1 \rightarrow t_2)</td>
<td>[2]</td>
</tr>
<tr>
<td></td>
<td><em>b</em> 340</td>
<td><em>b</em> 340</td>
<td><em>b</em> 340</td>
<td>(t_1 \rightarrow t_2)</td>
<td>[2]</td>
</tr>
<tr>
<td></td>
<td><em>b</em> 290</td>
<td><em>b</em> 290</td>
<td><em>b</em> 290</td>
<td>(t_1 \rightarrow t_2)</td>
<td>[2]</td>
</tr>
</tbody>
</table>

*This band shows vibrational progression with a separation of 740 cm\(^{-1}\). The peak position given here corresponds to the strongest peak in the progression.

a Room temperature.
b Liquid air/nitrogen temperature.
c Liquid helium temperature.
d Temperature between 4.2 and 77 K.

**References**


**Table 42. Optical absorption bands (in nm) of ferricyanide centers in alkali halides**

<table>
<thead>
<tr>
<th>Center</th>
<th>NaCl</th>
<th>KCl</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe(CN)₃⁻</td>
<td>505</td>
<td>500</td>
<td>(t_{2g}^2(t_{3g})^1(T_{1g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>420</td>
<td>414</td>
<td>(t_{2g}^1t_{2g}^1(T_{1u}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>376</td>
<td>377</td>
<td>(t_{2g}^2A_{1g}(^2A_{1g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>357</td>
<td>348</td>
<td>(t_{2g}^2(t_{4g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>338</td>
<td>323</td>
<td>(t_{2g}^1(t_{4g}, T_{1g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>302</td>
<td>296</td>
<td>(t_{1g}^1t_{2g}^1(t_{2g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>262</td>
<td>274</td>
<td>(t_{1g}^1(t_{2g}, T_{2g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>258</td>
<td>258</td>
<td>(t_{1g}^1t_{2g}^1t_{2g}^1)</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>248</td>
<td>248</td>
<td>(t_{1g}^1t_{2g}^1t_{2g}^1)</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>200</td>
<td>(t_{1g}^1t_{2g}^1t_{2g}^1)</td>
<td>[1]</td>
</tr>
</tbody>
</table>

a Room temperature.  
b Liquid air/nitrogen temperature.  
c Liquid helium temperature.  
d Temperature between 4.2 and 77 K.

**References**


**Table 43. Optical absorption bands (in nm) of cobalticyanide centers in alkali halides.**

<table>
<thead>
<tr>
<th>Center</th>
<th>NaCl</th>
<th>KCl</th>
<th>Assignment</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Co(CN)₃⁻</td>
<td>484</td>
<td>480</td>
<td>(t_{3g}^1(3T_{1g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>409</td>
<td>400</td>
<td>(t_{3g}^1(3T_{2g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>361</td>
<td>355</td>
<td>(t_{3g}^1(1T_{4g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>316</td>
<td>310</td>
<td>(t_{3g}^1(1T_{2g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>280</td>
<td>277</td>
<td>(t_{3g}^1(1T_{2g}))</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>260</td>
<td>258</td>
<td>(t_{1u})</td>
<td>[1]</td>
</tr>
<tr>
<td></td>
<td>201</td>
<td>201</td>
<td>(t_{1u})</td>
<td>[1]</td>
</tr>
</tbody>
</table>

a Room temperature.  
b Liquid air/nitrogen temperature.  
c Liquid helium temperature.  
d Temperature between 4.2 and 77 K.

**Reference**


25
PART II.

Vibrational Frequencies of Internal Modes of Complex Ions Doped in Alkali Halide Crystals
To succeed humanely in any complex, non-linear, dynamic, and uncertain situation a leader must be equipped with a creative and original intelligence.
Table 44. Point group symmetry, normal modes and their activity in infrared absorption and Raman scattering for the molecular ions investigated.

<table>
<thead>
<tr>
<th>No. of atoms</th>
<th>Point group symmetry</th>
<th>Modes and their symmetry and activity in infrared and Raman*</th>
<th>Molecular impurities investigated</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>D&lt;sub&gt;dh&lt;/sub&gt;</td>
<td>( \nu_6 (\Sigma_g^-; R) )</td>
<td>( \mathrm{N}_2^-, \mathrm{O}_2^-, \mathrm{S}_2^-, \mathrm{Se}_2^- )</td>
</tr>
<tr>
<td>2</td>
<td>C&lt;sub&gt;2v&lt;/sub&gt;</td>
<td>( \nu_4 (\Sigma_v^+; R) )</td>
<td>( \mathrm{OH}^-, \mathrm{OD}^-, \mathrm{CN}^-, \mathrm{SH}^-, \mathrm{SeH}^-, \mathrm{SSe}^- )</td>
</tr>
<tr>
<td>3</td>
<td>D&lt;sub&gt;sh&lt;/sub&gt;</td>
<td>( \nu_{12} (\Sigma_g^-; R) ) ( \nu_{20} (\Pi_u; IR) ) ( \nu_{33} (\Sigma_u^-; IR) )</td>
<td>( \mathrm{N}_2^-, \mathrm{BO}_2^- )</td>
</tr>
<tr>
<td>3</td>
<td>C&lt;sub&gt;wv&lt;/sub&gt;</td>
<td>( \nu_{13} (\Sigma_v^-; IR, R) ) ( \nu_{20} (\Pi; IR \ R) ) ( \nu_{33} (\Sigma_u^-; IR, R) )</td>
<td>( \mathrm{NCO}^-, \mathrm{NCS}^- )</td>
</tr>
<tr>
<td>3</td>
<td>C&lt;sub&gt;2v&lt;/sub&gt;</td>
<td>( \nu_{13} (A_1; IR, R) ) ( \nu_{20} (A_1; IR, R) ) ( \nu_{33} (B_2; IR, R) )</td>
<td>( \mathrm{NO}_2^-, \mathrm{NH}_2^-, \mathrm{ND}_2^-, \mathrm{H}_2\mathrm{O} \mathrm{NH}^-, \mathrm{S}_2^-, \mathrm{S}_3^-, \mathrm{S}_4^- )</td>
</tr>
<tr>
<td>4</td>
<td>C&lt;sub&gt;2v&lt;/sub&gt;</td>
<td>( \nu_{13} (A_1, IR, R) ) ( \nu_{20} (A_1; IR, R) ) ( \nu_{33} (E, IR, R) ) ( \nu_{4n} (E; IR, R) )</td>
<td>( \mathrm{ClO}_2^-, \mathrm{IO}_2^-, \mathrm{SeO}_2^2^- )</td>
</tr>
<tr>
<td>4</td>
<td>D&lt;sub&gt;2h&lt;/sub&gt;</td>
<td>( \nu_{13} (A'; R) ) ( \nu_{20} (A'; IR) ) ( \nu_{33} (E'; IR, R) ) ( \nu_{4b} (E'; IR, R) )</td>
<td>( \mathrm{NO}_2^-, \mathrm{CO}_2^-, \mathrm{BO}_3^- )</td>
</tr>
<tr>
<td>5</td>
<td>T&lt;sub&gt;d&lt;/sub&gt;</td>
<td>( \nu_{13} (A_1; R) ) ( \nu_{20} (E; R) ) ( \nu_{33} (T_2; IR, R) ) ( \nu_{4b} (T_2; IR, R) )</td>
<td>( \mathrm{NH}_2^-, \mathrm{ND}_2^-, \mathrm{BH}_2^-, \mathrm{BD}_2^-, \mathrm{BF}_2^- )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>( \mathrm{ClO}_2^-, \mathrm{MnO}_2^- \mathrm{SO}_2^2-, \mathrm{SeO}_2^2-, \mathrm{CrO}_2^+, \mathrm{MnO}_2^+, \mathrm{MoO}_2^+, \mathrm{BeF}_2^- )</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>O&lt;sub&gt;h&lt;/sub&gt;</td>
<td>( \nu_{13} (A_{18}; R) ) ( \nu_{36} (E_{6g}; R) ) ( \nu_{43} (T_{1u}; IR) )</td>
<td>( \mathrm{Co(CN)}_6^{3+}, \mathrm{Co(CN)}_6^{4-}, \mathrm{Co(CN)}_6^{4+}, \mathrm{Fe(CN)}_6^{2-}, \mathrm{Fe(CN)}_6^{3-}, \mathrm{Fe(CN)}_6^{3+} )</td>
</tr>
</tbody>
</table>

*Subscripts 's' and 'b' for the modes indicate stretching and bending respectively. IR and or R in the parenthesis after the modes means whether that particular mode is infrared and or Raman active.
Table 45. Internal vibration frequencies of homonuclear diatomic molecular ions doped in alkali halide crystals.

These ions have only one vibrational mode $v_s \left( \sum_y \right)$ which is Raman active and infrared inactive. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be $\pm 1$ cm$^{-1}$, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than $\pm 0.5$ cm$^{-1}$. ESR and uniaxial stress experiments$^1$ suggest that $O_\ell$, $S_\ell^-$ and $Se_\ell^-$ are aligned along (110) direction in FCC alkali halides.

<table>
<thead>
<tr>
<th>Crystal:Impurity</th>
<th>Frequency (cm$^{-1}$) $v_s \left( \sum_y \right)$</th>
<th>Temperature K</th>
<th>Remarks</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>KCl:N$_2^-$</td>
<td>1836 ± 3</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>KBr:N$_2^-$</td>
<td>1821 ± 3</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>Ki:N$_2^-$</td>
<td>1870 ± 3</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>NaCl:O$_2^-$</td>
<td>1144 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2, 3, 4]</td>
</tr>
<tr>
<td>NaBr:O$_2^-$</td>
<td>1131 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2, 3, 4]</td>
</tr>
<tr>
<td>KCl:O$_2^-$</td>
<td>1145 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2, 3, 4]</td>
</tr>
<tr>
<td>KBr:O$_2^-$</td>
<td>1135 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2, 3, 4]</td>
</tr>
<tr>
<td>Ki:O$_2^-$</td>
<td>1123 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2, 3, 4]</td>
</tr>
<tr>
<td>RbCl:O$_2^-\ell$</td>
<td>1141 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2, 3, 4]</td>
</tr>
<tr>
<td>RbBr:O$_2^-\ell$</td>
<td>1132 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2, 3, 4]</td>
</tr>
<tr>
<td>NaBr:S$_\ell^-\ell$</td>
<td>610 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>NaI:S$_\ell^-\ell$</td>
<td>592 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>KBr:S$_\ell^-\ell$</td>
<td>612 ± 2</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>Ki:S$_\ell^-\ell$</td>
<td>594±1</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>RbBr:S$_\ell^-\ell$</td>
<td>611 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>RbI:S$_\ell^-\ell$</td>
<td>598±1</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>NaI:Se$_\ell^-\ell$</td>
<td>333 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>Ki:Se$_\ell^-\ell$</td>
<td>325 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[2]</td>
</tr>
</tbody>
</table>

RT—Room temperature.

References

These ions have only one vibrational mode $\nu_s (\Sigma_g^+)$ which is both Raman and IR active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be $\pm 1 \text{ cm}^{-1}$, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than $\pm 0.5 \text{ cm}^{-1}$. Stress and dichroism experiments suggest that the molecular axis in the (100) direction for CN$^-$ and perhaps also for OH$^-$ in FCC alkali halides and (110) or possibly (111) in BCC alkali halides$^3$. The free ion frequencies are:

$$\nu_s = 3596 \text{ cm}^{-1} \text{ for OH}^-, \nu = 2680 \text{ cm}^{-1} \text{ for OD}^- \text{ and } \nu_s = 2042 \text{ cm}^{-1} \text{ for CN}^-.$$ 

<table>
<thead>
<tr>
<th>Crystal: Impurity</th>
<th>Frequency (cm$^{-1}$) $\nu_s (\Sigma_g^+)$</th>
<th>Temperature K</th>
<th>Remarks</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>NaCl:CN$^-$</td>
<td>2106.8</td>
<td>10</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>NaBr:CN$^-$</td>
<td>2087 ± 1</td>
<td>100</td>
<td>IR</td>
<td>[3]</td>
</tr>
<tr>
<td>NaI:CN$^-$</td>
<td>2074 ± 1</td>
<td>100</td>
<td>IR</td>
<td>[3]</td>
</tr>
<tr>
<td>KCl:CN$^-$</td>
<td>2087.7</td>
<td>8.5</td>
<td>Raman</td>
<td>[2]</td>
</tr>
<tr>
<td>KBr:CN$^-$</td>
<td>2078</td>
<td>2</td>
<td>IR</td>
<td>[4]</td>
</tr>
<tr>
<td>KI:CN$^-$</td>
<td>2067</td>
<td>2</td>
<td>IR</td>
<td>[4]</td>
</tr>
<tr>
<td>RbCl:CN$^-$</td>
<td>2081</td>
<td>2</td>
<td>IR</td>
<td>[4]</td>
</tr>
<tr>
<td>RbBr:CN$^-$</td>
<td>2070 ± 1</td>
<td>100</td>
<td>IR</td>
<td>[3]</td>
</tr>
<tr>
<td>RbI:CN$^-$</td>
<td>2063 ± 1</td>
<td>100</td>
<td>IR</td>
<td>[3]</td>
</tr>
<tr>
<td>CsCl:CN$^-$</td>
<td>2078 ± 1</td>
<td>100</td>
<td>IR</td>
<td>[3]</td>
</tr>
<tr>
<td>CsBr:CN$^-$</td>
<td>2066 ± 1</td>
<td>100</td>
<td>IR</td>
<td>[3]</td>
</tr>
<tr>
<td>CsI:CN$^-$</td>
<td>2053 ± 1</td>
<td>100</td>
<td>IR</td>
<td>[3]</td>
</tr>
<tr>
<td>NaCl:OH$^-$</td>
<td>3654.5 ± 0.5</td>
<td>4.5</td>
<td>IR</td>
<td>[6]</td>
</tr>
<tr>
<td>NaBr:OH$^-$</td>
<td>3626 ± 0.5</td>
<td>4.5</td>
<td>IR</td>
<td>[6]</td>
</tr>
<tr>
<td>KCl:OH$^-$</td>
<td>3641 ± 0.5</td>
<td>4.5</td>
<td>IR</td>
<td>[6]</td>
</tr>
<tr>
<td>KBr:OH$^-$</td>
<td>3618 ± 0.5</td>
<td>4.5</td>
<td>Raman and IR</td>
<td>[5, 6]</td>
</tr>
<tr>
<td>KI:OH$^-$</td>
<td>3603</td>
<td>4.5</td>
<td>IR</td>
<td>[6]</td>
</tr>
<tr>
<td>RbCl:OH$^-$</td>
<td>3632 ± 0.5</td>
<td>4.5</td>
<td>IR</td>
<td>[6]</td>
</tr>
<tr>
<td>NaCl:OD$^-$</td>
<td>2689</td>
<td>4.5</td>
<td>Raman</td>
<td>[5]</td>
</tr>
<tr>
<td>KCl:OD$^-$</td>
<td>2664.5 ± 0.5</td>
<td>4.5</td>
<td>IR</td>
<td>[6, 7]</td>
</tr>
<tr>
<td>KBr:OD$^-$</td>
<td>2668 ± 0.5</td>
<td>4.5</td>
<td>IR</td>
<td>[6]</td>
</tr>
<tr>
<td>KCl:SH$^-$</td>
<td>*2585</td>
<td>RT</td>
<td>IR</td>
<td>[8]</td>
</tr>
<tr>
<td>KBr:SH$^-$</td>
<td>*2569</td>
<td>RT</td>
<td>IR</td>
<td>[8]</td>
</tr>
<tr>
<td>KCl:SeH$^-$</td>
<td>*2294</td>
<td>RT</td>
<td>IR</td>
<td>[9]</td>
</tr>
<tr>
<td>NaI:SSe$^-$</td>
<td>462 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[10]</td>
</tr>
<tr>
<td>KI:SSe$^-$</td>
<td>464 ± 1</td>
<td>RT</td>
<td>Raman</td>
<td>[10]</td>
</tr>
</tbody>
</table>

RT Room temperature.

References

TABLE 47. Internal vibrational frequencies (cm\(^{-1}\)) of linear triatomic molecular ions with \(D_{\infty h}\) point group, doped in alkali halides.

These ions have one mode \(\nu_1\left(\sum_g s\right)\) which is only Raman active and two modes \(\nu_2\left(\Pi_g b\right)\) and \(\nu_3\left(\sum_g s\right)\) only infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be \(\pm 1\) cm\(^{-1}\), except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than \(\pm 0.5\) cm\(^{-1}\). \(N_\text{T}\) and \(BO_\text{T}\) enters substitutionally into the lattice at the anion site such that molecular axis is along (111) in FCC alkali halides [1, 2]. The free ion values are known only for \(N_\text{T}\) ions and are \(\nu_1 = 1344\) cm\(^{-1}\), \(\nu_2 = 645\) cm\(^{-1}\) and \(\nu_3 = 2041\) cm\(^{-1}\).

<table>
<thead>
<tr>
<th>Crystal : Impurity</th>
<th>Frequency (cm(^{-1}))</th>
<th>Temperature (K)</th>
<th>Remarks</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(\nu_1\left(\sum_g s\right))</td>
<td>(\nu_2\left(\Pi_g b\right))</td>
<td>(\nu_3\left(\sum_g s\right))</td>
<td></td>
</tr>
<tr>
<td>NaCl : (N_\text{T})</td>
<td>-</td>
<td>640.3 ± 0.1</td>
<td>2083.1 ± 0.1</td>
<td>120</td>
</tr>
<tr>
<td>NaBr : (N_\text{T})</td>
<td>-</td>
<td>-</td>
<td>2064.5</td>
<td>-</td>
</tr>
<tr>
<td>NaI : (N_\text{T})</td>
<td>-</td>
<td>-</td>
<td>2037.0</td>
<td>-</td>
</tr>
<tr>
<td>KCl : (N_\text{T})</td>
<td>-</td>
<td>643.0 ± 0.1</td>
<td>2051.2 ± 0.1</td>
<td>120</td>
</tr>
<tr>
<td>KBr : (N_\text{T})</td>
<td>-</td>
<td>641.5 ± 0.1</td>
<td>2038.2 ± 0.1</td>
<td>120</td>
</tr>
<tr>
<td>KI : (N_\text{T})</td>
<td>-</td>
<td>639.7 ± 0.1</td>
<td>2022.1 ± 0.1</td>
<td>120</td>
</tr>
<tr>
<td>RbCl : (N_\text{T})</td>
<td>-</td>
<td>-</td>
<td>2040.0</td>
<td>-</td>
</tr>
<tr>
<td>RbBr : (N_\text{T})</td>
<td>-</td>
<td>-</td>
<td>2029.0</td>
<td>-</td>
</tr>
<tr>
<td>RbI : (N_\text{T})</td>
<td>-</td>
<td>-</td>
<td>2016.2</td>
<td>-</td>
</tr>
<tr>
<td>CsCl : (N_\text{T})</td>
<td>-</td>
<td>-</td>
<td>2043.0</td>
<td>-</td>
</tr>
<tr>
<td>CsBr : (N_\text{T})</td>
<td>-</td>
<td>-</td>
<td>2026.0</td>
<td>-</td>
</tr>
<tr>
<td>CsI : (N_\text{T})</td>
<td>-</td>
<td>-</td>
<td>2006.0</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{16}\text{O}^{16}\text{O}) : (BO_\text{T})</td>
<td>-</td>
<td>610</td>
<td>2043</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{16}\text{O}^{17}\text{O})</td>
<td>-</td>
<td>-</td>
<td>2038</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{18}\text{O}^{16}\text{O})</td>
<td>-</td>
<td>-</td>
<td>2029</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{18}\text{O}^{18}\text{O})</td>
<td>-</td>
<td>590</td>
<td>1972</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{16}\text{O}^{17}\text{O})</td>
<td>-</td>
<td>-</td>
<td>1968</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{18}\text{O}^{15}\text{O})</td>
<td>-</td>
<td>-</td>
<td>1959</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{16}\text{O}^{16}\text{O}) : (BO_\text{T})</td>
<td>-</td>
<td>607</td>
<td>2029</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{18}\text{O}^{17}\text{O})</td>
<td>-</td>
<td>-</td>
<td>2023</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{18}\text{O}^{19}\text{O})</td>
<td>-</td>
<td>-</td>
<td>2016</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{18}\text{O}^{19}\text{O})</td>
<td>-</td>
<td>587</td>
<td>1959</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{16}\text{O}^{17}\text{O})</td>
<td>-</td>
<td>-</td>
<td>1953</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{16}\text{O}^{18}\text{O})</td>
<td>-</td>
<td>-</td>
<td>1946</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{16}\text{O}^{16}\text{O}) : (BO_\text{T})</td>
<td>-</td>
<td>607</td>
<td>2016</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{16}\text{O}^{16}\text{O})</td>
<td>-</td>
<td>-</td>
<td>2000</td>
<td>-</td>
</tr>
<tr>
<td>(^{10}\text{B}^{16}\text{O}^{16}\text{O})</td>
<td>-</td>
<td>587</td>
<td>1946</td>
<td>-</td>
</tr>
</tbody>
</table>

References

These ions have three modes, $\nu_1(\Sigma^+)$, $\nu_2(\Pi)$, and $\nu_3(\Sigma^+)$ which are both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be $\pm 1$ cm$^{-1}$, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than $\pm 0.3$ cm$^{-1}$. NCO$^-$ and NCS$^-$ enter the alkali halide lattice substitutionally replacing the anion such that the molecular axis is along (111) in FCC alkali halides [1] and along (100) in BCC alkali halides [5]. The free ion frequencies are:

\[ \nu_1 = 1207 \text{ cm}^{-1}, \quad \nu_2 = 637, 628 \text{ cm}^{-1} \text{ and } \nu_3 = 2165 \text{ cm}^{-1} \text{ for NCO}^-, \]

and $\nu_1 = 743 \text{ cm}^{-1}, \quad \nu_2 = 470 \text{ cm}^{-1} \text{ and } \nu_3 = 2066 \text{ cm}^{-1} \text{ for NCS}^-.$

<table>
<thead>
<tr>
<th>Crystal : Impurity</th>
<th>Frequency (cm$^{-1}$)</th>
<th>Temperature K</th>
<th>Remarks</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\nu_1(\Sigma^+)$</td>
<td>$\nu_2(\Pi)$</td>
<td>$\nu_3(\Sigma^+)$</td>
<td></td>
</tr>
<tr>
<td>NaCl: NCO$^-$</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{14}$N$^{13}$C$^{16}$O$^-$</td>
<td>633.2 ± 0.3</td>
<td>2211.2 ± 0.3</td>
<td>298</td>
<td>IR</td>
</tr>
<tr>
<td>$^{14}$N$^{13}$C$^{16}$O$^-$</td>
<td>633.2 ± 0.3</td>
<td>2211.2 ± 0.3</td>
<td>298</td>
<td>IR</td>
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<td>IR</td>
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<td>2182</td>
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<td>IR</td>
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<tr>
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<td>2170</td>
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</tr>
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<td>2170</td>
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<td>298</td>
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<td>2170</td>
<td>298</td>
<td>IR</td>
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<tr>
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<td>1211.8</td>
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<td>2187</td>
<td>100</td>
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<td>CsI: NCO$^-$</td>
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<td>630</td>
<td>2170</td>
<td>100</td>
</tr>
<tr>
<td>NaI: NCS$^-$</td>
<td></td>
<td></td>
<td></td>
<td>IR</td>
</tr>
<tr>
<td>KI: NCS$^-$</td>
<td></td>
<td></td>
<td></td>
<td>IR</td>
</tr>
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<td>Rbl: NCS$^-$</td>
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<td></td>
<td>IR</td>
</tr>
<tr>
<td>CsI: NCS$^-$</td>
<td></td>
<td></td>
<td></td>
<td>IR</td>
</tr>
</tbody>
</table>

References

Table 49. Vibrational frequencies (cm\(^{-1}\)) of bent triatomic molecular ions doped in alkali halides.

These ions have three modes \(\nu_1(A_1), \nu_2(A_1)\) and \(\nu_3(B_2)\) which are both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be \(\pm 1\) cm\(^{-1}\), except in the cases marked with an asterisk where no idea of accuracy could be obtained. The NO\(_2^+\) ion enters substitutionally into the lattice at the anion site such that the 2-fold axis of the ion points in the (110) directions in FCC alkali halides. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than \(\pm 0.5\) cm\(^{-1}\). The free ion values are:

\[
\begin{align*}
\nu_1 &= 1328\text{ cm}^{-1}, \quad \nu_2 = 828.2\text{ cm}^{-1} \text{ and } \nu_3 = 1261\text{ cm}^{-1} \text{ for NO}\(_2^+\) \\
\nu_1 &= 3210\text{ cm}^{-1}, \quad \nu_2 = 1532\text{ cm}^{-1} \text{ and } \nu_3 = 3266\text{ cm}^{-1} \text{ for NH}_2^+ \\
\nu_1 &= 2355\text{ cm}^{-1}, \quad \nu_2 = 1131\text{ cm}^{-1} \text{ and } \nu_3 = 2429\text{ cm}^{-1} \text{ for ND}_2^+ \\
\nu_1 &= 2387\text{ cm}^{-1}, \quad \nu_2 = 1247\text{ cm}^{-1} \text{ and } \nu_3 = 3236\text{ cm}^{-1} \text{ for NH}_2^- \text{ and} \\
\nu_1 &= 3657\text{ cm}^{-1}, \quad \nu_2 = 1595\text{ cm}^{-1} \text{ and } \nu_3 = 3756\text{ cm}^{-1} \text{ for H}_2\text{O.}
\end{align*}
\]

<table>
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<tr>
<th>Crystal:Impurity</th>
<th>Frequency (cm(^{-1}))</th>
<th>Temperature K</th>
<th>Remarks</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>(\nu_1(A_1))</td>
<td>(\nu_2(A_1))</td>
<td>(\nu_3(B_2))</td>
<td></td>
</tr>
<tr>
<td>NaCl:NO(_2^+)</td>
<td>1346</td>
<td>636</td>
<td>1304</td>
<td>2</td>
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<tr>
<td>NaBr:NO(_2^+)</td>
<td>1327 ± 2</td>
<td>828 ± 2</td>
<td>1283 ± 2</td>
<td>6</td>
</tr>
<tr>
<td>KCl:NO(_2^+)</td>
<td>1329</td>
<td>805</td>
<td>1290</td>
<td>2</td>
</tr>
<tr>
<td>KBr:NO(_2^+)</td>
<td>1316.2 ± 0.5</td>
<td>798.1 ± 0.5</td>
<td>1275 ± 0.5</td>
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<tr>
<td>KIO(_2^+)</td>
<td>1303.9 ± 0.5</td>
<td>779 ± 0.5</td>
<td>1256.6 ± 0.5</td>
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<tr>
<td>RbCl:NO(_2^+)</td>
<td>1294.2 ± 0.5</td>
<td>793 ± 0.5</td>
<td>1249.5 ± 0.5</td>
<td>8</td>
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<tr>
<td>KI:NO(_2^+)</td>
<td>1308</td>
<td>806 ± 2</td>
<td>1253</td>
<td>5</td>
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<td>NaCl:SF(_2^-)</td>
<td>531 ± 1</td>
<td>-</td>
<td>-</td>
<td>300</td>
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<tr>
<td>NaBr:SF(_2^-)</td>
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<tr>
<td>KCl:SF(_2^-)</td>
<td>527 ± 1</td>
<td>-</td>
<td>540 ± 2</td>
<td>300</td>
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<tr>
<td>KBr:SF(_2^-)</td>
<td>532 ± 1</td>
<td>-</td>
<td>585 ± 2</td>
<td>300</td>
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<tr>
<td>KI:SF(_2^-)</td>
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<td>RbCl:SF(_2^-)</td>
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<td>300</td>
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<td>RbBr:SF(_2^-)</td>
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<td>544 ± 1</td>
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<td>KBr:NH(_2^-)</td>
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<td>KCl:NHD(_-)</td>
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<td>KBr:NHD(_-)</td>
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<td>1330</td>
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<tr>
<td>KCl:ND(_2^-)</td>
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<td>1137</td>
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</tr>
<tr>
<td>KBr:ND(_2^-)</td>
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<td>1113</td>
<td>2395</td>
<td>20</td>
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<td>3435</td>
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<td>3400</td>
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<tr>
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<tr>
<td>KI:H(_2)O</td>
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<td>1690</td>
<td>3390</td>
<td>20</td>
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*aThe absorption maxima expressed in eV in the paper is converted to wave number (cm\(^{-1}\)) by using the conversion factor 1 eV = 8065 cm\(^{-1}\).

References

These ions have four modes $\nu_1(A_1), \nu_2(A_1), \nu_3(E)$ and $\nu_4(E)$ which are both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be $\pm 1 \text{ cm}^{-1}$, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than $\pm 0.5 \text{ cm}^{-1}$. ClO$_3^-$, IO$_3^-$ and SeO$_4^{2-}$ ions go substitutionally into the lattice at the anion site such that the 3-fold axis of the ion coincides with (111) direction in FCC alkali halides. The free ion frequencies are:

$$
\begin{align*}
\nu_1 &= 930, \ \nu_2 = 610, \ \nu_3 = 982 \quad \text{and} \quad \nu_4 = 479 \text{ cm}^{-1} \\
\nu_1 &= 754, \ \nu_2 = 373, \ \nu_3 = 774 \quad \text{and} \quad \nu_4 = 355, 330 \text{ cm}^{-1} \\
\nu_1 &= 807, \ \nu_2 = 432, \ \nu_3 = 737 \quad \text{and} \quad \nu_4 = 374 \text{ cm}^{-1} \\
\end{align*}
$$

for ClO$_3^-$, IO$_3^-$ and SeO$_4^{2-}$. The data is presented in Table 50:

<table>
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<tr>
<th>Crystal:Impurity</th>
<th>Frequency (cm$^{-1}$)</th>
<th>Temperature K</th>
<th>Remarks</th>
<th>References</th>
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<td>1027.5</td>
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<td>$^{37}\text{ClO}_3^-$</td>
<td>1017.5</td>
<td>-</td>
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<td>1016</td>
<td>-</td>
<td>IR [1]</td>
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<td>$^{37}\text{ClO}_3^-$</td>
<td>1006</td>
<td>-</td>
<td>IR [1]</td>
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<td>947.60</td>
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<td>$^{37}\text{ClO}_3^-$</td>
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<td>930.80</td>
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<td>$^{18}\text{IO}_3^-$</td>
<td>791.05 ± 0.15</td>
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<td>749.75 ± 0.15</td>
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<td>767.25 ± 0.15</td>
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<td>$^{35}\text{SeO}_4^{2-}$</td>
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<td>763 ± 1</td>
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<td>$^{35}\text{SeO}_4^{2-}$</td>
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<td>752.5 ± 1</td>
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<td>$^{35}\text{SeO}_4^{2-}$</td>
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<td>749 ± 1</td>
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* Charge compensating defect occupying the nearest neighbour positions lowers the site symmetry of the ion resulting in the splitting of $\nu_3$.

References

Table 51. Vibrational frequencies (cm\(^{-1}\)) of planar tetraatomic molecular ions \((D_{3h})\) doped in alkali halide crystals.

These ions have four modes \(\nu_1(A')\) Raman active, \(\nu_2(A'')\) infrared active and \(\nu_3(E')\) and \(\nu_4(E')\) both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be \(\pm 1\) cm\(^{-1}\), except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than \(\pm 0.5\) cm\(^{-1}\).

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<th>Remarks</th>
<th>References</th>
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<td>(\nu_2(A''))</td>
<td>(\nu_3(E'))</td>
<td>(\nu_4(E'))</td>
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<td>---</td>
<td>---</td>
<td>1423 ±1</td>
<td>---</td>
</tr>
<tr>
<td>NaBr: NO(_3^-)</td>
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<td>---</td>
<td>1390 ±1</td>
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<td>NaI: NO(_3^-)</td>
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<tr>
<td>KCl: NO(_3^-)</td>
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<td>---</td>
<td>1398 ±1</td>
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</tr>
<tr>
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<td>(^{14})N(_{16})O(_3^-)</td>
<td>1054.8 ±0.5</td>
<td>814.3 ±0.5</td>
<td>1382.2 ±0.5</td>
</tr>
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<td>(^{14})N(<em>{16})O(</em>{18})O(_2^-)</td>
<td>1034.9</td>
<td>837.8</td>
<td>1383.2</td>
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<tr>
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<td>(^{14})N(<em>{16})O(</em>{18})O(_2^-)</td>
<td>944.4</td>
<td>830.6</td>
<td>1363.4</td>
</tr>
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<td>1055.1</td>
<td>820.0</td>
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</tr>
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<td>KI: NO(_3^-)</td>
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<td>816.4</td>
<td>1352.3</td>
</tr>
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<td>KCl: CO(_3^-)</td>
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<td>---</td>
<td>882</td>
<td>1476</td>
</tr>
<tr>
<td>KCl: CO(_3^-), Ca(^{2+})</td>
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<td>---</td>
<td>1520</td>
<td>1398</td>
</tr>
<tr>
<td>KCl: CO(_3^-), Sr(^{2+})</td>
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<td>880</td>
<td>1493</td>
<td>1398</td>
</tr>
<tr>
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<td>864</td>
<td>1551</td>
<td>1333</td>
</tr>
<tr>
<td>KBr: CO(_3^-)</td>
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<td>---</td>
<td>883</td>
<td>1475</td>
</tr>
<tr>
<td>KBr: CO(_3^-), Pb(^{2+})</td>
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<td>863</td>
<td>1555</td>
<td>1319</td>
</tr>
<tr>
<td>KI: CO(_3^-)</td>
<td>---</td>
<td>---</td>
<td>885</td>
<td>1485</td>
</tr>
<tr>
<td>KBr: BO(_3^-)</td>
<td>952</td>
<td>735</td>
<td>1247</td>
<td>1398</td>
</tr>
<tr>
<td>KBr: H(_3)BO(_3)</td>
<td>1040</td>
<td>---</td>
<td>1450</td>
<td>1368</td>
</tr>
</tbody>
</table>

*Because of the charge compensating defect in the neighbourhood of the ion the symmetry is lowered resulting in the splitting of \(\nu_3\) and \(\nu_4\).*
TABLE 52. Vibrational frequencies of penta-atomic tetrahedral molecular ions ($T_d$) doped in alkali halides.

These ions have four modes of which $\nu_i(A_1)$ and $\nu_i(E)$ are only Raman active, while $\nu_i(T_2)$ and $\nu_i(T_2)$ are both Raman and infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be $\pm 1$ cm$^{-1}$, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wave-number unless the accuracy is equal to or better than $\pm 0.5$ cm$^{-1}$. These tetrahedral ions enter the lattice substitutionally such that the four bonds are directed along the (111) directions in FCC alkali halides [2, 3]. In BCC alkali halides the tetrahedral ions occupy the anion site such that the site symmetry is reduced to $D_{4d}$ [1–3]. The free ion frequencies are:

$$
\begin{align*}
\nu_1 &= 3040, \nu_2 = 1680, \nu_3 = 3145 \text{ and } \nu_4 = 1400 \text{ cm}^{-1} \text{ for } ^{14}\text{NH}_4^+ \\
\nu_2 &= 1215, \nu_3 = 2346 \text{ and } \nu_4 = 1065 \text{ cm}^{-1} \text{ for } ^{18}\text{BF}_4^- \\
\nu_1 &= 2204, \nu_2 = 1210, \nu_3 = 2244 \text{ and } \nu_4 = 1080 \text{ cm}^{-1} \text{ for } ^{14}\text{BH}_4^- \\
\nu_1 &= 1770, \nu_2 = 935, \nu_3 = 1696 \text{ and } \nu_4 = 823 \text{ cm}^{-1} \text{ for } ^{18}\text{BD}_4^- \\
\nu_1 &= 769, \nu_2 = 353, \nu_3 = 984 \text{ and } \nu_4 = 524 \text{ cm}^{-1} \text{ for } ^{10}\text{BF}_4^- \\
\nu_1 &= 769, \nu_2 = 353, \nu_3 = 1016 \text{ and } \nu_4 = 529 \text{ cm}^{-1} \text{ for } ^{18}\text{BF}_4^- \\
\nu_1 &= 928, \nu_2 = 459, \nu_3 = 1119 \text{ and } \nu_4 = 625 \text{ cm}^{-1} \text{ for } ^{18}\text{ClO}_4^- \\
\nu_1 &= 845, \nu_2 = 355, \nu_3 = 910 \text{ and } \nu_4 = 395 \text{ cm}^{-1} \text{ for } ^{14}\text{MnO}_4^- \\
\nu_1 &= 983, \nu_2 = 450, \nu_3 = 1105 \text{ and } \nu_4 = 611 \text{ cm}^{-1} \text{ for } ^{18}\text{SO}_4^- \\
\nu_1 &= 833, \nu_2 = 335, \nu_3 = 875 \text{ and } \nu_4 = 422 \text{ cm}^{-1} \text{ for } ^{14}\text{SeO}_4^2- \\
\nu_1 &= 847, \nu_2 = 348, \nu_3 = 884 \text{ and } \nu_4 = 368 \text{ cm}^{-1} \text{ for } ^{18}\text{CrO}_4^2- \\
\nu_1 &= 894, \nu_2 = 381, \nu_3 = 833 \text{ and } \nu_4 = 318 \text{ cm}^{-1} \text{ for } ^{18}\text{MoO}_4^2-
\end{align*}
$$

<table>
<thead>
<tr>
<th>Crystal:Impurity</th>
<th>Frequency ($\text{cm}^{-1}$)</th>
<th>Temperature K</th>
<th>Remarks</th>
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<td>$\nu_1(A_1)$</td>
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<td>2278 $\pm$ 3</td>
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<td>1707 $\pm$ 3</td>
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<td>1079 $\pm$ 0.5</td>
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<td>538.0 $\pm$ 0.5</td>
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<td>1090.5 $\pm$ 0.5</td>
<td>536.5 $\pm$ 0.5</td>
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References

### Table 52. Vibrational frequencies of penta-atomic tetrahedral molecular ions ($T_d$) doped in alkali halides.—Continued

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<th>Crystal:Impurity</th>
<th>Frequency (cm$^{-1}$)</th>
<th>Temperature K</th>
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<td>$\nu_1(A_1)$</td>
<td>$\nu_2(E)$</td>
<td>$\nu_3(T_2)$</td>
<td>$\nu_4(T_2)$</td>
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<td>KBr:BF$_4$</td>
<td>1124.0 ± 0.5</td>
<td>532.5 ± 0.5</td>
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<tr>
<td>KBr:BF$_4$</td>
<td>1084.0 ± 0.5</td>
<td>531.0 ± 0.5</td>
<td>300</td>
<td>IR</td>
</tr>
<tr>
<td>KI:BF$_4$</td>
<td>1116.5 ± 0.5</td>
<td>528.0 ± 0.5</td>
<td>300</td>
<td>IR</td>
</tr>
<tr>
<td>KI:BF$_4$</td>
<td>1076.5 ± 0.5</td>
<td>526.5 ± 0.5</td>
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<td>IR</td>
</tr>
<tr>
<td>CsBr:BF$_4$</td>
<td>1120 ± 1</td>
<td>535 ± 1</td>
<td>300</td>
<td>IR</td>
</tr>
<tr>
<td>CsBr:BF$_4$</td>
<td>1080 ± 1</td>
<td>533 ± 1</td>
<td>300</td>
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</tr>
<tr>
<td>CsI:BF$_4$</td>
<td>1109 ± 1</td>
<td>529 ± 1</td>
<td>300</td>
<td>IR</td>
</tr>
<tr>
<td>CsI:BF$_4$</td>
<td>1070 ± 1</td>
<td>527 ± 1</td>
<td>300</td>
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<tr>
<td>KCl:ClO$_4^-$</td>
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<td>KBr:ClO$_4^-$</td>
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<td>RbBr:ClO$_4^-$</td>
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<td>631.78</td>
<td>176</td>
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<tr>
<td>RbI:ClO$_4^-$</td>
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<td>634.78</td>
<td>176</td>
<td>IR</td>
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<td>RbI:ClO$_4^-$</td>
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<td>631.36</td>
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<td>KBr:MnO$_4^-$</td>
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<td>KI:MnO$_4^-$</td>
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<td>913 ± 1</td>
<td>300</td>
<td>IR, R</td>
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<td>RbBr:MnO$_4^-$</td>
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<td>923.5</td>
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<td>KCl:SO$_4^{2-}$, Ca$^{2+}$</td>
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<td>1157</td>
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<td>bIR</td>
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<td>KCl:SO$_4^{2-}$, Zn$^{2+}$</td>
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<td>KCl:SO$_4^{2-}$, Ba$^{2+}$</td>
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<td>KCl:SO$_4^{2-}$, Pb$^{2+}$</td>
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<td>1185</td>
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<td>KCl:SO$_4^{2-}$, Cd$^{2+}$</td>
<td>1185</td>
<td>1156</td>
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<td>KCl:SO$_4^{2-}$, Cd$^{2+}$</td>
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<td>KCl:SO$_4^{2-}$, Pb$^{2+}$</td>
<td>969</td>
<td>1197</td>
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Table 52. Vibrational frequencies of penta-atomic tetrahedral molecular ions \((T_a)\) doped in alkali halides. — Continued

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<tr>
<th>Crystal:Impurity</th>
<th>Frequency ((cm^{-1}))</th>
<th>Temperature (K)</th>
<th>Remarks</th>
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<tr>
<td>KBr:SO(_4^{2-}), Ca(^{2+})</td>
<td>(975) --- 1172 ---</td>
<td>77</td>
<td>bIR</td>
<td>[9]</td>
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<tr>
<td>(34)SO(_4^{2-})</td>
<td>977 --- 1185 ---</td>
<td>77</td>
<td>bIR</td>
<td>[9]</td>
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<tr>
<td>KCl:SeO(_4^{2-}), M(^{2+})</td>
<td>(80)SeO(_4^{2-})</td>
<td>925.5 ± 1 904.5 ± 1 860.5 ± 1</td>
<td>120</td>
<td>bIR</td>
</tr>
<tr>
<td>(80)SeO(_4^{2-})</td>
<td>836 --- 928 ± 1 907 ± 1 862.5 ± 1</td>
<td>120</td>
<td>bIR</td>
<td>[11]</td>
</tr>
<tr>
<td>(78)SeO(_4^{2-})</td>
<td>--- --- 930.5 ± 1 909.5 ± 1 865.0 ± 1</td>
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<td>bIR</td>
<td>[11]</td>
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<tr>
<td>(77)SeO(_4^{2-})</td>
<td>--- --- 931.5 ± 1 910.5 ± 1 866.0 ± 1</td>
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<td>[11]</td>
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<td>(78)SeO(_4^{2-})</td>
<td>--- --- 933 ± 1 912 ± 1 867.5 ± 1</td>
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<td>[11]</td>
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<td>KBr:SeO(_4^{2-}), M(^{2+})</td>
<td>(85)SeO(_4^{2-})</td>
<td>917.5 ± 1 897.5 ± 1 851.5 ± 1</td>
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<tr>
<td>(80)SeO(_4^{2-})</td>
<td>828.5 --- 920 ± 1 899.5 ± 1 854 ± 1</td>
<td>120</td>
<td>bIR</td>
<td>[12]</td>
</tr>
<tr>
<td>(78)SeO(_4^{2-})</td>
<td>--- --- 922.5 ± 1 902.0 ± 1 856.0 ± 1</td>
<td>120</td>
<td>bIR</td>
<td>[11]</td>
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<tr>
<td>(77)SeO(_4^{2-})</td>
<td>--- --- 924 ± 1 903 ± 1 857 ± 1</td>
<td>120</td>
<td>bIR</td>
<td>[11]</td>
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<td>(78)SeO(_4^{2-})</td>
<td>--- --- 925.5 ± 1 904.5 ± 1 858.5 ± 1</td>
<td>120</td>
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<td>[11]</td>
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<tr>
<td>KCl:CrO(_4^{2-})</td>
<td>--- --- 913 ± 1</td>
<td>300</td>
<td>IR</td>
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<tr>
<td>KCl:CrO(_4^{2-}),□</td>
<td>860 --- 939 ± 1 896 ± 1 887 ± 1</td>
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<td>Temperature K</td>
<td>Remarks</td>
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<tr>
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<td>$v_1$ (A₁)</td>
<td>$v_2$ (E)</td>
<td>$v_3$ (T₂)</td>
<td>$v_4$ (T₂)</td>
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<tr>
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<td>944 ± 1</td>
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<td>KBr : CrO₃⁻</td>
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<td>KBr : CrO₃⁻, □</td>
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<td>927 ± 1</td>
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<td>KBr : CrO₃⁻, Mg²⁺</td>
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<td>---</td>
<td>937 ± 1</td>
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<tr>
<td>KBr : CrO₃⁻, Sr²⁺</td>
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<td>938 ± 1</td>
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<td>KBr : CrO₃⁻, Ba²⁺</td>
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<td>KBr : CrO₃⁻, Pb²⁺</td>
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<td>907</td>
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<tr>
<td>KI : CrO₄⁻, □</td>
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<td>926 ± 1</td>
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<tr>
<td>KI : CrO₄⁻, Ca²⁺</td>
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<tr>
<td>KBr : MnO₄⁻, □</td>
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<td>870 ± 1</td>
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<td>890 ± 1</td>
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<td>KBr : MoO₄⁻</td>
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<tr>
<td>KBr : MoO₄⁻, □</td>
<td>898</td>
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<td>876 ± 1</td>
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### Table 52. Vibrational frequencies of penta-atomic tetrahedral molecular ions (T₄) doped in alkali halides. — Continued

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<th>Crystal:Impurity</th>
<th>Frequency (cm⁻¹)</th>
<th>Temperature K</th>
<th>Remarks</th>
<th>References</th>
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<td>ν₃(T₂)</td>
<td>ω₄(T₂)</td>
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<td>910.4 ± 1</td>
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<td>870.4 ± 1</td>
<td>770.0 ± 1</td>
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<tr>
<td>KCl:BeF²⁺.Ca²⁺</td>
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<td>853.4 ± 1</td>
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<td>KCl:BeF²⁺.Ba²⁺</td>
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<td>909.0 ± 1</td>
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<td>869.0 ± 1</td>
<td>780.0 ± 1</td>
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<td>KCl:BeF²⁺.Zn²⁺</td>
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<td>910.1 ± 1</td>
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<td>870.0 ± 1</td>
<td>770.0 ± 1</td>
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<tr>
<td>KCl:BeF²⁺.Cd²⁺</td>
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<td>910.8 ± 1</td>
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<td>870.0 ± 1</td>
<td>770.0 ± 1</td>
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<tr>
<td>KCl:BeF²⁺.Sn²⁺</td>
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<td>----</td>
<td>910.1 ± 1</td>
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<td></td>
<td>870.0 ± 1</td>
<td>770.0 ± 1</td>
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<td></td>
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<tr>
<td>KCl:BeF²⁺.Pb²⁺</td>
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<td>909.8 ± 1</td>
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<tr>
<td></td>
<td>868.0 ± 1</td>
<td>757.6 ± 1</td>
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* Here the charge compensation is by an anion vacancy in one of the twelve nearest neighbour anion sites, reducing the symmetry from T₄ to C₄v, resulting in the splitting of ν₃(T₂) into ν₃(A'') + ν₃(A') + ν₃(A'''). Here ν₃(A''') < ν₃(A'). □ denotes anion vacancy.

b Here charge compensation is by a divalent cation in one of the six nearest neighbour cation sites, reducing the symmetry of the ion to C₂v, resulting in the splitting of ν₃(T₂) into ν₃(A₁) + ν₃(B₁) + ν₃(B₂). Here ν₃(B₂) > ν₃(A₁) > ν₃(B₁). Mn²⁺ denotes unknown divalent cation impurity.

### References


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Vibrational frequencies of octahedral complexes doped in alkali halide crystals.

The $v_1(A_{1g})$ and $v_3(E_u)$ stretching modes are only Raman active and the stretching mode $v_6(T_{1u})$ is only infrared active. The accuracy, when given by the authors, is quoted. In other cases the accuracy is estimated to be $\pm 1$ cm$^{-1}$, except in the cases marked with an asterisk where no idea of accuracy could be obtained. The values have been rounded off to nearest wavenumber unless the accuracy is equal to or better than $\pm 0.5$ cm$^{-1}$. Co(CN)$_6^{3-}$ and Fe(CN)$_6^{3-}$ ($n = 3, 4, 5$) ions enters the lattice substitutionally such that the metal ion occupies the cation site and the six CN$^-$ ions occupying the six nearest neighbour anion sites in FCC alkali halides.

<table>
<thead>
<tr>
<th>Crystal : Impurity</th>
<th>$v_1(A_{1g})$</th>
<th>$v_3(E_u)$</th>
<th>$v_6(T_{1u})$</th>
<th>Temperature K</th>
<th>Remarks</th>
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Table 53. Vibrational frequencies of octahedral complexes doped in alkali halide crystals—Continued

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a Since there are charge compensating defects in the neighbourhood of the ions, the symmetry of the complex is lowered resulting in the splitting of $\nu_9(T_{1u})$ mode giving rise to more than one band.

b These species are produced by X-irradiating the NaCl and KCl crystals containing Co(CN)$_6^{2-}$ and Fe(CN)$_6^{2-}$ ions.

References

PART III.

External Vibrational Frequencies of Impurity Centers Doped in Alkali Halide Crystals
Table 54a. Frequencies of external modes (in cm⁻¹) due to U-centers in alkali halides

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<th>RbBr</th>
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<th>CsBr</th>
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<td>b 498</td>
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a Room temperature.  b Liquid air/nitrogen temperature.  c Liquid helium temperature.  d Temperature between 4.2 and 77 K.
References


Table 54b. Frequencies of external modes (in cm\(^{-1}\)) due to point impurities in alkali halides

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48
### Table 54b. Frequencies of external modes (in \text{cm}^{-1}) due to point impurities in alkali halides—Continued

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\textsuperscript{a} Room temperature.
\textsuperscript{b} Liquid air/nitrogen temperature.
\textsuperscript{c} Liquid helium temperature.
\textsuperscript{d} Temperature between 4.2 and 77 K.

### References

Table 55a. Frequencies of external modes (in cm\(^{-1}\)) due to molecular impurities in alkali halides

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* Room temperature.

b Liquid air/nitrogen temperature.

\(^{c}\) Liquid helium temperature.

\(^{d}\) Temperature between 4.2 and 77 K.

References

Table 55b. Frequencies of external modes (in cm⁻¹) due to OH⁻ and OD⁻ in alkali halides

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<td>c 86</td>
<td>c 77</td>
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<td>[4, 5]</td>
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a Room temperature.
b Liquid air/nitrogen temperature.
c Liquid helium temperature.
d Temperature between 4.2 and 77 K.

References

**Title and Subtitle:**
Electronic Absorption and Internal and External Vibrational Data of Atomic and Molecular Ions Doped in Alkali Halide Crystals

**Authors:**
S.C. Jain, A.V.R. Warrier, and S.K. Agarwal

**Abstract:**
Spectral data for more than 70 atomic and molecular ions doped in alkali halide crystals are tabulated. The tables include electronic absorption data, listings of internal vibrational frequencies of doped complex ions, and tabulations of the frequencies of external modes. The data that appear in the tables were selected on the basis of the consistency among different authors, the types of instruments, and the temperature of measurement. In addition to the data, the tables include the spectroscopic assignments given by the authors in the references cited.

**Key Words:**
Atomic ions; doped alkali halide crystals; external vibrational modes; internal vibrational modes; molecular ions.

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