Dative Bonding Between Closed-Shell Atoms: The BeF⁻ Anion

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Beryllium: Chemistry’s Littlest Rule Breaker

- Beryllium is known to exhibit unexpectedly strong attractive forces under conditions where it is considered a closed shell atom:
  - Be₂⁺ dimer
  - He-BeO
- Understanding abnormal bonding with beryllium can:
  1. Improve theoretical models
  2. Push the bounds of our fundamental chemical understanding.
- BeF⁻ anion has only been studied theoretically, with a suggested bond energy of 342 kJ/mol.²
- In our work, we seek to provide experimental confirmation of the bonding in BeF⁻.

Confirmation of Bonding in BeF⁻

Table 1. Electron affinities (EA), vibrational frequencies (ω₁), and bond dissociation energies (D₀) for BeF and BeF⁻. All values are given in wavenumbers (cm⁻¹).

<table>
<thead>
<tr>
<th>Compound</th>
<th>EA</th>
<th>ω₁</th>
<th>D₀</th>
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<tbody>
<tr>
<td>BeF</td>
<td>8697 ± 6</td>
<td>8692</td>
<td>47480</td>
</tr>
<tr>
<td>BeF⁻</td>
<td>8189</td>
<td>45443</td>
<td></td>
</tr>
</tbody>
</table>

Tunable laser set to 1734 cm⁻¹ (570.2 nm)

Velocity Map Imaging Photoelectron Spectroscopy

VMI Instrument:

Adjustment of molecular beam by ion optics
Imaging of electrons via velocity map imaging (VMI) optics and camera
Laser ablation and mass separation of ions

What we are imaging:

electron kinetic energy (eKE) detection range
Tunable laser
Neutral Ground State
Electron binding energy (eBE) for 0→0 transition
Anion Ground State

- Electrons are removed from the anion using a high energy photon (hv) from a pulsed laser.
- Any energy that is not used in the photodetachment process is imparted to the removed electron as kinetic energy (eKE).
- All electrons with the same eKE are mapped to the same distance, r, from the center of the detector screen.
- Images are converted into spectra, and electron binding energies (eBE), or the A → A transition energies, are determined by subtracting the eKE from the known laser energy.

References


Acknowledgements

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Future Directions: Diving Deeper

Confirmation of dative bonding in BeF⁻ introduces the question: What characteristics of beryllium allow for this phenomenon?

- electron-correlation
- excited state participation
- Be polarizability
- Lewis acidity of Be

By understanding what makes beryllium unique, we can better refine our knowledge of chemical bonding, in general.