３原子分子クラスターイオン内における分子間共有結合の形成と、その電子・幾何構造の研究
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Summary

- Dimer ion core structure.
- The semi-covalent bond formed in dimer ion core.

C₂O₂⁺ changes structure with cluster size:
- C₂O₂⁺: bent structure
- C₂O₂⁺ structure
- Structure in exp. and calc. different for C₂O₂⁺

Characteristic of solvent molecules
- Broad nature of HOMO of OCS.
- Weaker intermolecular interaction.

IRPD spectra of (CO₂)ₙ⁺
- Intensity decreases with increasing n.
- Band position not coincident with that of CO₂.
- C₂O₂⁺ ion core

IRPD spectra of (OCS)ₙ⁺ and (CS₂)₂n⁺
- Band position almost the same as that of CO₂.
- Solvent CO₂ molecules

Structure of C₂O₂⁺
- Structure of dimer is determined by balance between two factors.

Structure and Band Number for Dimer
- IR activity of dimer ions
- C₂ symmetry

Q1: Why structure of C₃O₄⁺ alternately changes?
Q2: Why bare C₂O₂⁺ has bent (C₃) structure?
Q3: Why structure different between exp. and calc. for C₃S⁺?

A1: Rather C₂O₂⁺ has hardest structure.
Structural change of C₂O₂⁺ in (CO₂)ₙ⁺
- structural weakness of C₂O₂⁺
- characteristics of solvation

Proposed structural change:
- Internal bonds formed between solvent and ion core.
- Solvent complex bonded asymmetrical to ion core.

A2: Due to broad nature of HOMO of OCS.

PES along out-of-plane torsional motion
- PES shallow → weaker intermolecular interaction
- Calculation cannot reproduce correctly the PES.

A3: Due to weaker interaction in C₃S⁺.

Experimental
- IR spectra of cluster ions can be measured as a function of cluster size.