Ab Initio Assessment of the Bonding in Disulfonates Containing Divalent Nitrogen and Phosphorus Atoms

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The iminodisulfonate, \([\text{N(SO}_3\text{)}_2]^{3-}\), and phosphinodisulfonate, \([\text{P(SO}_3\text{)}_2]^{3-}\), ions have been investigated by performing ab initio MP2/6-311+G** calculations. The nitrogen and phosphorus atoms as part of the ions are shown to be divalent with a negative charge and two lone pairs on the nitrogen and phosphorus atoms. The experimentally known calcium sodium iminodisulfonate trihydrate and the analogous unknown compound calcium sodium phosphinodisulfonate trihydrate have also been investigated using the MP2/6-311+G** calculations. For the nitrogen compound, only minor changes occur in the iminodisulfonate ion when it becomes part of the calcium sodium iminodisulfonate trihydrate. For the phosphorus compound, the geometry of the phosphinodisulfonate ion changes significantly as part of calcium sodium phosphinodisulfonate trihydrate. Furthermore, the charges associated with the atoms in calcium sodium phosphinodisulfonate trihydrate are quite different from those of the phosphinodisulfonate ion. For calcium sodium iminodisulfonate trihydrate, the Raman spectrum has been measured, and it compares well with the spectrum derived using HF/6-311+G** calculations.

General information
Publication status: Published
Organisations: Physical and Biophysical Chemistry, Department of Chemistry
Contributors: Andersen, V. B., Berg, R. W., Shim, I.
Pages: 4447-4455
Publication date: 2017
Peer-reviewed: Yes

Publication information
Journal: ACS Omega
Volume: 2
Issue number: 8
Ratings:
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.02 SJR 0.749 SNIP 0.524
Original language: English
Keywords: Electronic structure, Molecular structure, Molecular vibration, Quantum mechanics, Spectra, Vibrational frequency
Electronic versions:
acsomega.7b00266.pdf
DOIs:
10.1021/acsomega.7b00266

Bibliographical note
This is an open access article published under an ACS AuthorChoice License.
Source: FindIt
Source ID: 2372979484
Research output: Contribution to journal › Journal article – Annual report year: 2017 › Research › peer-review