

Charge density distribution in aminomethylphosphonic acid.

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Rok wydania

2010

Czasopismo

Acta Crystallographica
Section B: Structural
Science, Crystal Engineering
and Materials

Numer woluminu

B66

Strony

559-567

DOI

10.1107/S0108768110026091

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The experimental charge density distribution in aminomethylphosphonic acid has been determined from X-ray diffraction and its topological features have been analyzed. The results have shown that the P—O bonds are highly polarized, moreover the P—OH bond is weaker than the bonds to unprotonated O atoms. These facts have been confirmed by theoretical density functional theory (DFT) calculations, which have shown that the single, strongly polarized bonds within the phosphonate group are modified by hyperconjugation effects.

Słowa kluczowe

charge density distribution, aminophosphonic acid, density functional calculations, hyperconjugation, Electronic structure

Adres publiczny

<https://doi.org/10.1107/S0108768110026091>