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Charge-density distribution in sodium bis(4-nitrophenyl)phosphate.

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Streszczenie

The electron-density distribution in sodium bis(4-nitrophenyl)phosphate has been analyzed using the multipole refinement of X-ray diffraction data and of theoretical density-functional theory (DFT) calculations. The ester P-O bonds are particularly long and their topological parameters (density at the bond critical point, Laplacian) are lower than for other P-O bonds. Some disagreement between the experimental and theoretical charges of atoms constituting the nitro groups has been observed and the possible reasons are discussed. Weak polarization effects produced by sodium cations may be observed within the phosphate fragment; they are more manifest in the case of the nitro groups.

Adres publiczny

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