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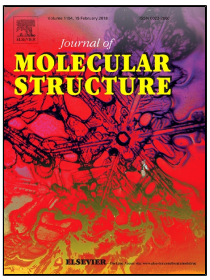

Syntheses, spectroscopic properties and molecular structure of silver phytate complexes - IR, UV-VIS studies and DFT calculations.

A. Zając, L. Dymińska, J. Lorenc, M. Ptak, J. Hanuza

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Highlights

- The spectroscopic properties of three silver phytates of the formulae IP6Ag, $IP6Ag_2$ and $IP6Ag_3$ were compared to non-complexing IP6 phytic acid.
- We report new data on the role of intra- and inter-molecular interactions in the structure of phytic acid and its complexes.
- It was found that it is C_s in non-substituted $H_2PO_4^-$ anion but the substitution of Ag^+ ions leads to lowering the symmetry to C_1.
- The symptoms of the Fermi resonance were found in the spectra.