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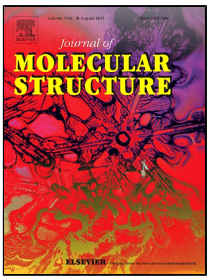

A novel coordination polymer of 7-Azaindole-3-carboxylic acid with sodium ions: crystal and molecular structures, vibrational spectra and DFT calculations

Barbara Morzyk-Ociepa, Ksenia Szmigiel, Rafał Petrus, Ilona Turowska-Tyrk, Danuta Michalska

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Highlights

A novel coordination polymer of 7-Azaindole-3-carboxylate ion with Na(I) was obtained.

7AI3CAH2 acts as bridging ligand binding Na(I) via one carboxylate O and the Npy atom.

The monoatomic bridging mode of the 7-azaindole moiety involving Npy atom is unusual.

A single crystal XRD, IR, Raman and DFT studies confirmed the structure of the complex.

A detailed interpretation of the IR and Raman spectra of the Na(I) complex is reported.