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On the acid-base properties of pyrazine-2-thiocarboxamide and its complexes with Fe(II), Cu(II), Zn(II) and Ni(II) in polar solvents.

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Streszczenie

Acid-base properties of 1,4-diazine-2-thiocarboxamide (*PTCA*) most stable conformers were studied as well as its complexes with Fe(II), Cu(II), Zn(II) and Ni(II) in water, acetonitrile, methanol and ethanol solvents. All studies were performed by means of theoretical density functional method (DFT), and the solvents were modeled as a polarizable continuum. Due to significant differences in stability two groups of conformers can be distinguished. Only one group, containing amino group, shall be observed experimentally. Full four-stage protonation and two-stage deprotonation maps of PTCA have been revealed. The 1:1 and 2:1 series of complexes have been found with Fe(II), Cu(II), Zn(II) and Ni(II) cations. General complexation enthalpy characteristic was found as: $\Delta H_{298_Cu2+} > \Delta H_{298_Ni2+} \gg \Delta H_{298_Cu2+} \gg \Delta H_{298_Zn2+}$, and $\Delta H_{298_ethanol} > \Delta H_{298_acetonitrile} > \Delta H_{298_mehtanol} > \Delta H_{298_water}$.

Słowa kluczowe

Pyrazine-2-thiocarboxamide (PTCA), Deprotonation, Metal complexes, DFT

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